- 21-23 July 2022-

INTERNATIONAL CONFERENCE ON CARBON CAPTURE SCIENCE AND TECHNOLOGY 2022

Online

CCST 2022 CONFERENCE

Organisation

Queen's University Belfast

Co-Organisation

Tsinghua University

Zhejiang University

Chongqing University

Chair

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Professor Xin Tu, University of Liverpool
Professor Luciana Porto de Souza Vandenberghe, Federal University of Parana
Professor Meihong Wang, The University of Sheffield,
Professor Haiping Yang, Huazhong University of Science and Technology

DAY 1

-Day ONE

Plenary 1 and Opening

(Link of meeting room) (Link of koushare)

UK Time	Speaker		Title
12:40-13:00	Opening + CCST Leader & Future Star Awards		
13:00-13:40	PL-1	Professor Yushan Yan (University of Delaware)	Anion exchange membrane based electrochemical direct air capture systems
13:40-14:10	Social activities & gifts		

Main meeting room and Session A TEAMs link & 蔻享 link

Session B TEAMs link & 蔻享 link

Session C TEAMs link & 蔻享 link

(Session links are also available at the beginning of each session)

Social activities link (Wonder.me)

Day TWO – Parallel Session A

(Link of meeting room) (Link of koushare)

UK Time		Chair:	Dr Changlei Qin
		Speaker	Title
8:20-9:00	PL-2	Professor Jun Cheng (Chongqing University)	Research and development of CO_2 reduction with microalgae from coal-fired flue gas in China
9:00-9:40	PL-5	Professor Mengxiang Fang (Zhejiang University)	Development of flue gas CO_2 chemical absorption technology
9:40-10:00		*Break & social activities (Wonder.me link)*	
		Chairs:	Dr Jin Huang & Dr Jian Shen
10:00-10:25	KA-1	Dr Shijian Lu (China University of Mining and Technology)	Economic analysis and application potential of CO_2 capture technology for industrial tail gas – KA-1
10:25-10:40	OA-1	Muhammad Usman Azam (The University of Aberdeen)	Waste plastic management using circular economy via hydro catalytic route
10:40-10:55	OA-2	William Davies (Brunel University London)	Machine Learning in CCUS and Blue Hydrogen Production: Pros and Cons
10:55-11:10	IA-1	Lewis McDonald (University of Bath)	Mineral Carbonation for Industrial Decarbonisation of Portland Cement and Additives
11:10-11:25	OA-3	Ruikai Zhao (Tianjin University)	Temperature swing adsorption for carbon dioxide capture: adsorbent material, adsorption chamber and experimental system
11:25-11:40	OA-4	Yuanyuan Wang (Queen's University Belfast)	Application of CNT prepared from waste plastic to phase change materials for battery thermal management
11:40-12:00		*Break & social activities (Wonder.me link)*	

DAY 2

CCST 2022 CONFERENCE

		Chairs:	Professor Ningbo Gao & Dr Daxin Liang
12:00-12:25	KA-2	Professor Daniel C. W. Tsang (The Hong Kong Polytechnic University)	Customized Design of Iron-Manganese Oxide Clusters on Biochar Composites
12:25-12:40	OA-5	Srigan N. Moharir (Imperial College London)	Novel Tungsten doped Iron Oxide as an oxygen carrier for Chemical Looping Combustion
12:40-12:55	OA-6	Salman Masoudi Soltani (Brunel University London)	Cost effective waste-derived adsorbents for post-combustion carbon capture
12:55-13:10	IA-2	Wen Liu (Nanyang Technological University)	A novel supercritical CO_2 based natural gas fuelled power cycle for ultrahigh efficiency energy generation with inherent carbon capture
13:10-13:25	OA-7	Yuanting Qiao (University of Sheffield)	Techno-economic Analysis of Integrated Carbon Capture and Utilisation compared with Carbon Capture and Utilisation
13:25-13:40	OA-8	Han Yi (Kangwon National University)	Application of carbon capture and storage technology in ultra-high performance concrete
13:40-14:10	Break, social activities & gifts (*Wonder.me link*)		
		Chairs:	Dr Yuhe Cao & Dr Asim Khan
14:10-14:35	KA-3	Professor Haiqing Lin (University at Buffalo)	Metal Ion-Coordinated Supramolecular Polymer Networks for Post-combustion Carbon Capture
14:35-14:50	OA-9	Weining Li (China University of Petroleum (East China))	High-Performance Single and Bimetallic Desulfurization Adsorbents with Abundant Active Sites Prepared from Phytoremediation
14:50-15:05	OA-10	Elfina Azwar (Universiti Malaysia Terengganu)	Solvothermal liquefaction of waste Kariba weed into value-added products
15:05-15:20	IA-3	Professor Chunfeng Song Tianjin University	Development of Cryogenic CO_2 capture technologies

15:20-15:40	KA-4	Dr Katherine Mary Hornbostel (University of Pittsburgh)	Ocean Carbon Capture Using Membrane Contactors
15:40-15:55	OA-20	Cristhian Molina Fernández (UCLouvain)	Biocatalytic composite membranes for CO_2 capture

Day TWO – Parallel Session B

(Link of meeting room) (Link of koushare)

UK Time	Presentation No.	Chair:	Dr Shuai Deng
		Speaker	Title
8:20-9:00	PL-3	Professor Liyuan Deng (Norwegian University of Science and Technology)	Efficient Membranes for CO_2 Capture: Paths towards Industrial Applications
9:00-9:40	PL-6	Professor Zhi Wang (Tianjin University)	Development of pilot CO_2 capture membrane system
9:40-10:00		*Break & social activities (Wonder.me link)*	
		Chairs:	Dr Xuezhong He & Dr Chunhai Yi
10:00-10:25	KB-1	Professor Zhen Fang (Nanjing Agricultural University)	Pretreatment and hydrolysis of lignocellulosic Biomass for Biorefineries
10:25-10:40	OB-1	Boyu Li (Tongji University)	Insights into solvent effect guiding the fabrication of highly performance mixed-matrix membrane for CO_2 separation
10:40-10:55	OB-2	Hui Shen LAU (Xiamen University Malaysia)	Functionalized two-dimensional g-C_3N_4 nanosheets in PIM-1 mixed matrix membranes for gas separation
10:55-11:10	IB-1	G.A. Mutch (Newcastle University)	Challenges for supported molten-carbonate membranes
11:10-11:25	OB-3	Junyao Wang (Guangdong University of Technology)	Water-energy-carbon nexus: A life cycle assessment of post-combustion carbon capture technology from power plant level

DAY 2

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11:25-11:40	OB-4	Huanhao Chen (Nanjing Tech University)	Integration of Membrane Separation with Non-Thermal Plasma (NTP) Catalysis: A Proof-of-Concept for CO_2 Capture and Utilisation (CCU)
11:40-12:00	*Break & social activities (Wonder.me link)*		
		Chairs:	Prof. Xinying Liu & Dr Aneta Magdziarz
12:00-12:25	KB-2	Professor Xiaohua Ma (Tiangong University)	Ultra-selective membranes obtained by pre-oxidation of intrinsic microporous polymers for natural gas sweetening
12:25-12:40	OB-5	Shaohan Lian (Tianjin University)	Construction of Asymmetric Mixed Matrix Membranes Based on Ionic Liquids and Characteristics of CO_2 Separation
12:40-12:55	OB-6	Jing wei (Sichun University)	High-performance CO_2 separation membranes developed by non-solvent induced molecular rearrangement
12:55-13:10	IB-2	A. L. Khan COMSATS University Islamabad	Current trends and future directions in membrane based CO_2 capture
13:10-13:25	OB-7	Chen Zhang (Queen's University Belfast)	Direct air capture of CO_2 by KOH activated bamboo biochar
13:25-13:40	IB-3	Jude Onwudili (Aston University)	Production of aromatic carboxylic acids from CO_2 and biomass-derived-phenolic compounds
13:40-14:10	*Break, social activities & gifts (Wonder.me link)*		
		Chairs:	Dr Zhien Zhang & Dr Zhikun Zhang
14:10-14:35	KB-3	Dr Francesco Barzagli (National Research Council)	Innovative CO_2 capture processes based on nonaqueous amine sorbents and solid acid catalysts for low-temperature regeneration
14:35-14:50	OB-9	Yash Girish Shah (National Energy Technology Laboratory)	Multiphase reacting flow modeling of MEA-based CO_2 absorption in packed columns
14:50-15:05	OB-10	Fraser Norris (University of Strathclyde)	Density functional theory investigation into catalytic hydrocarbon adsorption and dissociation for carbon nanotube nucleation

15:05-15:20	IB-4	Xiangzhou Yuan (Korea University)	Closing both carbon and plastic loops towards a circular economy
15:20-15:35	OB-11	Zilong Liu (China University of Petroleum-Beijing)	Charge-modulated adsorption and separation of CO_2 over N_2 on carbon nitride nanosheets: Insights from GCMC simulations
15:35-15:50	OB-12	Wenqi Xu (Norwegian university of science and technology)	Enhanced CO_2/H_2 separation by GO and PVA-g-GO embedded PVAm nanocomposite membranes

Day TWO – Parallel Session C

(Link of meeting room) (Link of koushare)

UK Time	Presentation No.	Chair:	Dr Hui Zhou
		Speaker	Title
8:20-9:00	PL-4	Professor Jun Huang (University of Sydney)	Catalyst development for sustainable fuel & chemical production from CO_2
9:00-9:40	PL-7	Professor Christoph Müller (ETH Zurich)	CO_2 capture and conversion: Materials, Activity and Stability
9:40-10:00		*Break & social activities (Wonder.me link)*	
		Chairs:	Dr Melis Duyar & Dr Jiawei Wang
10:00-10:25	KC-1	Dr Tiancun Xiao (University of Oxford)	Commercialization of Lab Research in Catalysis, A Journey for Job Creation and Decarbonization Mission
10:25-10:40	OC-1	Khushbu G. Patel (Rai University)	A review on role of Ruthenium (Ru) based catalyst in CO_2 Capture and hydrogenation reactions
10:40-10:55	OC-2	Jing Dai (Nankai University)	Hydrotalcite derived NiFe alloys anchored on periclase-phase (Mg, Al)O_x nanosheets for CO_2 reforming of toluene assisted by DBD plasma

DAY 2

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10:55-11:10	IC-1	Shaojun Xu (Cardiff University)	Integrated one-step CO_2 adsorption-conversion process by non-thermal plasma
11:10-11:25	OC-3	Yuqi zhang (Hebei University of Technology)	Study on synthesis catalyst of municipal Solid waste incineration bottom ash for dry reforming of methane
11:25-11:40	OC-4	Dingshan Cao (Huazhong University of Science and Technology)	Dry reforming of methane by $LaNiO_3$ perovskite oxide: influence of preparation methods and research on regeneration properties
11:40-12:00	*Break & social activities (Wonder.me link)*		
		Chairs:	**Dr Hongman Sun & Dr Dingding Yao**
12:00-12:25	KC-2	Dr Hui Zhou (Tsinhua University)	2D molybdenum carbide (MXene) for CO_2 hydrogenation
12:25-12:40	OC-5	Guoping Hu (Ganjiang Innovation Academy)	CO_2 absorption using carbonate solvent with a bio-inspired temperature responsive promoter
12:40-12:55	OC-6	Yalou Guo (The University of Melbourne)	Capture and enrichment of low- grade methane by dual-reflux vacuum swing adsorption
12:55-13:10	IC-2	Hongman Sun (China University of Petroleum (East China))	CaO-based Materials for Integrated CO_2 Capture and Utilization
13:10-13:25	OC-7	Shengshen Gu (Changzhou University)	In-situ Polymerization of cobalt porphyrin on carbon nanotubes for efficient electrochemical CO_2 reduction
13:25-13:40	OC-8	Yuanling Li (Nankai University)	Plasma-catalytic dry reforming of methane over Ni/boron nitride catalysts
13:40-14:10	*Break, social activities & gifts (Wonder.me link)*		
		Chairs:	**Dr Katherine Mary Hornbostel & Dr Shouliang Yi**
14:10-14:35	KC-3	Michael Matuszewski (CEO and Founder of AristoSys)	The Evolution of Carbon Capture

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14:35-14:50	OC-9	Fanhou Kong (Queen's University Belfast)	Effect of Boron Anomaly and Multi-electron Reactions on Lithiation Process of Amorphous Cathodes
14:50-15:05	OC-10	Xueru Wang (Xi'an Jiaotong University)	Effects of Amine Functional Groups and Microporous Structures on CO_2 absorption performance of anion exchange resin
15:05-15:20	IC-3	X.-Y. Yu (Oak Ridge National Laboratory)	In situ molecular imaging of green solvents for CO_2 capture
15:20-15:35	OC-11	Muhammad Ibrahim Irshad (University of Hull)	Computational catalyst design for solvent regeneration in post-combustion CO_2 capture (PCC) process
15:35-15:50	OC-12	Eni Oko (Newcastle University)	Study of water-lean solvents for the post-combustion CO_2 capture process

DAY 3

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Day THREE – Parallel Session A

(Link of meeting room) (Link of koushare)

UK Time	Presentation No.	Speaker	Title
		Chair:	Dr Yeshui Zhang
8:00-8:40	PL-8	Professor Meihong Wang (University of Sheffield)	Systems Engineering for Carbon Capture and Utilisation in the context of CCUS
8:40-9:05	KA-7	Dr Changlei Qin (Chongqin University)	Construction of Efficient and Low-Cost Li4SiO4 and the Integrated CO_2 Capture/Conversion by DRM
9:05-9:20	OA-11	John Olusoji Owolabi (University of Hull)	Modelling and Analysis of Catalysts-aided Solvent Regeneration in Post-Combustion CO_2 Capture Process
9:20-9:40		*Break & social activities (Wonder.me link)*	
		Chair:	Dr Yikai Xu
9:40-10:05	KA-5	Professor Yatao Zhang (Zhengzhou University)	Rational design of mixed-matrix silver complex membranes for propylene/propane separation
10:05-10:20	OA-12	Liu Wei (Zhejiang University)	Analysis of carbon capture from a coal-fired power plant integrating heat pump technology
10:20-10:35	OA-13	Chang Geng (Ningxia University)	ReaxFF study on CLC behavior of N-PACs with different N microchemical environments in CuO oxygen carriers
10:35-10:50	IA-4	Xuezhong He (Guangdong Technion-Israel Institute of Technology)	Techno-economic Feasibility Analysis of Carbon Membranes for Integrated Biohydrogen Purification and CO_2 Capture
10:50-11:05	OA-14	Siew Kei Lau (Xiamen University Malaysia)	Comparative life cycle assessment on metal-organic frameworks production for CO_2 capture
11:05-11:25		*Break & social activities (Wonder.me link)*	
		Chair:	Dr Wen Liu

DAY 3

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11:25-11:40	OA-15	Yuxuan Gao Nanjing Normal University)	Hydrothermal Synthesis of CuS Catalysts for Electrochemical CO_2 Reduction
11:40-11:55	OA-16	Dharmjeet Madhav (KU Leuven)	Bio-inspired CO_2 capture and simultaneous mineralization using polydopamine as crystal growth modifier in an aqueous system
11:55-12:10	OA-17	Hewen Li (Nanjing Normal University)	Stabilized CO_2 capture performance of Zr-supported CaO-based sorbents synthesized by a facile and rapid combustion method
12:10-12:25	OA-18	Zhikun Zhang (Hebei University of Technology)	Fabrication of incineration bottom ash-derived CaO-based sorbent with self-enhanced CO_2 capture capacity and stability
12:25-12:40	IA-5	Yongqing Xu (Huazhong University of Science and Technology)	Structure and surface insight into a temperature-sensitive CaO-based CO_2 sorbent
12:40-13:10		*Break, social activities & gifts (Wonder.me link)*	
		Chair:	Dr Jiawei Wang
13:10-13:35	KA-6	Zhongde Dai (Sichuan University)	Polymeric membranes for CO_2 capture: from lab to industry
13:35-13:50	OA-19	Fan Chen (Texas A&M University)	Rational Design of Mixed Matrix Membranes with Metal-Organic Polyhedra for CO2/N2 separation

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Day THREE – Parallel Session B

(Link of meeting room) (Link of koushare)

UK Time	Presentation No.	Chair:	Dr Chunfei Wu
		Speaker	Title
8:00-8:40	PL-9	Professor Peter Robertson (Queen's University Belfast) Professor	The photocatalytic reduction of carbon dioxide – a materials or a reactor engineering challenge?
8:40-9:05	KB-4	Professor Canghai Ma (Dalian University of Technology)	Design and fabrication of advanced membranes for CO_2 separation
9:05-9:20	OB-13	Shuzhuang Sun (Queen's University Belfast and Hainan university)	Ni promoted Fe-CaO dual functional materials for integrated CO_2 capture and reverse water-gas shift reaction
9:20-9:40	*Break & social activities (Wonder.me link)*		
		Chair:	Dr Yongqing Xu
9:40-10:05	KB-5	Dr Qilei Song (Imperial College London)	Microporous polymer membranes for gas separation and energy storage
10:05-10:20	OB-14	Long Jiang (Zhejiang University)	Water effect on adsorption carbon capture in metal organic framework: a molecular simulation
10:20-10:35	OB-15	Jiangtao Liu (University of Science and Technology of China)	Polymers of intrinsic microporosity for CO_2 separation and capture
10:35-10:50	IB-5	Cui Quan (Xi'an Jiaotong University)	Amine-impregnated silica zeolite from microalgae ash at different calcination temperatures for CO_2 capture
10:50-11:05	OB-16	Hailong Li (Central South University)	Development of Li_4SiO_4 pellets using extrusion–spheronization technique for cyclic CO_2 capture
11:05-11:25	*Break & social activities (Wonder.me link)*		
		Chair:	Guoping Hu
11:25-11:40	OB-17	Jiapeng Wang (Southeast University)	Enhancement of the production of hydrocarbon-rich fuel and high-quality bio-oil from corn stalk by Na2S2O8 pretreatment combined with rapid pyrolysis

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11:40-11:55	OB-18	Mingzhe Sun (The Hong Kong Polytechnic University)	Transition metal cation-exchanged SSZ-13 zeolites for CO_2 capture and separation from N_2
11:55-12:10	OB-19	Ming Zhang (China University of Petroleum(East China))	Molecular simulation of CO_2 capture in amine-modified zeolite 13X
12:10-12:25	IB-6	Leiqing Hu (University at Buffalo)	Molecularly engineering polybenzimidazole for efficient pre-combustion CO_2 capture
12:25-12:40	OB-21	Svenja Vogt (Technische Hochschule Mittelhessen)	Accelerated carbonation of concrete slurries and recycled aggregates for the alleviation of the carbon footprint
12:40-13:10		*Break, social activities & gifts (Wonder.me link)*	
		Chair:	Dr Xiaolei Fan
13:10-13:50	PL-11	Peijun Hu (Queen's University Belfast)	Some recent theoretical progresses in heterogeneous catalysis

DAY 3

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Day THREE – Parallel Session C

(Link of meeting room) (Link of koushare)

UK Time	Presentation No.	Speaker	Title
		Chair:	Dr Hui Zhou
8:00-8:40	PL-10	Profesor Haiping Yang (Huazhong University Science and Technology)	Biomass Pyrolysis for Biochar and Its High-value Utilization
8:40-9:05	KC-4	Professor Su Shiung Lam (University Malaysia Terengganu)	Sustainable CO_2 capture via adsorption by chitosan-based functional biomaterial derived from biorefinery application: a review on recent advances, challenges, and future prospects
9:05-9:20	OC-13	Dominik Horváth (University of Pannonia)	Municipal solid waste pyrolysis-gasification over zeolite and eggshell supported catalysts for modification of hydrogen/carbon monoxide ratio
9:20-9:40		*Break & social activities (Wonder.me link)*	
		Chair:	Dr Qian Xu
9:40-10:05	KC-5	Dr Haresh Manyar (Queen's University Belfast)	Emerging Technologies for Net Zero World and Beyond
10:05-10:20	OC-14	Maria Elena Lozano Fernandez (University of Pannonia)	Carbon dioxide looping on biochar obtained from sewage sludge pyrolysis-gasification
10:20-10:35	OC-15	Godknows Dziva (Tianjin University)	Process design of hydrogen-enriched gas production through two-stage sorption-enhanced biomass gasification
10:35-10:50	OC-21	Qi Huang (Queen's University Belfast)	Enhanced Efficiency of Photo Switching Metal-Organic Framework Toward Low Energy Carbon Dioxide Capture
10:50-11:05	OC-16	Yunsong Yu (Xi'an Jiaotong University)	Atom solution to capture carbon dioxide at low temperature
11:05-11:25		*Break & social activities (Wonder.me link)*	
		Chair:	Dr Shijian Lu

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11:25-11:40	OC-17	Niranchana Rajamanickam (PSNA College of Engineering & Technology)	Carbon Capture and its storage - A deeper insight
11:40-11:55	OC-18	Joni Jupesta (Research Institute of Innovative Technology for the Earth (RITE))	Modelling the technoeconomic and life cycle assessment of the bioenergy carbon capture and storage (BECCS) in Southeast Asia
11:55-12:10	OC-19	Ying Ji (Zhejiang University)	CO_2 Adsorption of Amine-Based Coconut Shell Activated Carbon: Equilibrium, Kinetics and Competitive Adsorption
12:10-12:25	OC-20	Yuandong Yang (Shandong University)	One-step fabrication of size-controllable, biowaste-templated Li_4SiO_4 spheres via freeze-drying method for cyclic CO_2 capture
12:25-12:40	IC-5	Shijie Yu (Tsinghua University)	Hydrothermal conversion of pectin under a temperature-pressure independent process
12:40-13:10		*Break, social activities & gifts (Wonder.me link)*	
		Chair:	Dr Long Jiang
13:10-13:50	PL-12	Professor Robert (Bob) Farrauto (Columbia University)	Dual Function Materials, comprised of monolithic supported mixtures of catalyst and sorbent, for direct air capture of 400 ppm CO_2 in ambient air followed by catalytic methanation: The impact realistic condition

Plenary 13 and closing

(Link of meeting room) (Link of koushare)

13:50-14:30	PL-13	Christopher Jones (Georgia Tech)	Development and Deployment of Negative Emissions Technologies (NETs): Direct Air Capture (DAC) as Humanity's Moonshot for the 21st Century
14:30-15:00		Award + Closing ceremony	

Plenary Speaker

PL-1 Prof. Yushan Yan, University of Delaware

PL-2 Prof. Jun Cheng, Chongqing University

PL-3 Prof. Liyuan Deng, Norwegian University of Science and Technology

PL-4 Prof. Jun Huang, University of Sydney

PL-5 Prof. Mengxiang Fang, Zhejiang University

PL-6 Prof. Zhi Wang, Tianjin University

PL-7 Prof. Christoph Müller, ETH Zurich

PL-8 Prof. Meihong Wang, University of Sheffield

PL-9 Prof. Peter Robertson, Queen's University Belfast

PL-10 Prof. Haiping Yang, Huazhong University Science and Technology

PL-11 Prof. Peijun Hu, Queen's University Belfast

PL-12 Prof. Robert (Bob) Farrauto, Columbia University

PL-13 Prof. Christopher Jones, Georgia Tech

Keynote Speaker

KA-1 Dr. Shijian Lu, China University of Mining and Technology

KA-2 Prof. Daniel C. W. Tsang, The Hong Kong Polytechnic University

KA-3 Prof. Haiqing Lin, University at Buffalo

KA-4 Dr. Katherine Mary Hornbostel, University of Pittsburgh

KA-5 Prof. Yatao Zhang, Zhengzhou University

KA-6 Dr. Zhongde Dai, Sichuan University

KA-7 Dr. Changlei Qin, Chongqing University

KB-1 Prof. Zhen Fang, Nanjing Agricultural University

KB-2 Prof. Xiaohua Ma, Tiangong University

KB-3 Dr. Francesco Barzagli, National Research Council

KB-4 Prof. Canghai Ma, Dalian University of Technology

KB-5 Dr. Qilei Song, Imperial College London

KC-1 Dr. Tiancun Xiao, University of Oxford

KC-2 Dr. Hui Zhou, Tsinghua University

KC-3 Dr. Michael Matuszewski, CEO and Founder of AristoSys

KC-4 Prof. Su Shiung Lam, University Malaysia Terengganu

KC-5 Dr. Haresh Manyar, Queen's University Belfast

Invited Speaker

IA-1 Dr. Lewis McDonald, University of Bath

IA-2 Dr. Wen Liu, Nanyang Technological University

IA-3 Dr. C. Song, Tianjin University

IA-4 Dr. Xuezhong He, Guangdong Technion-Israel Institute of Technology

IA-5 Dr. Yongqing Xu, Huazhong University of Science and Technology

IB-1 Dr. G.A. Mutch, Newcastle University

IB-2 Dr. A. L. Khan, COMSATS University Islamabad

IB-3 Dr. Jude Onwudili, Aston University

IB-4 Dr. X. Yuan, Korea University

IB-5 Dr. Cui Quan, Xi,an Jiaotong University

IB-6 Dr. Leiqing Hu, University at Buffalo

IC-1 Dr. Shaojun Xu, Cardiff University

IC-2 Dr. Hongman Sun, China University of Petroleum (East China)

IC-3 Dr. X.-Y. Yu, Oak Ridge National Laboratory

IC-5 Dr. Shijie Yu, Tsinghua University

CCST2022 supporting organisations

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 823745.

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- Session maximum 50 persons, circle maximum 15 persons
- Using desktop or iPad can move around to join or invite to a new conversation and walk away to quit
- Using mobile devices please click session or circle list and use top list to approach people for circle conversations
- You can lock your current circle to prevent others join your conversation, if you lock and leave, you will not be allowed to go back
- You can click and message privately to a single person
- A circle admin can invite and remove from list
- Share-screen is allowed on desktop computers but not supported on tablets or mobile devices

Raffles

In the social activities, we will provide gifts to participants who will be **r**andomly picked using online software.

Please enter your name into one of the following documents. We will then copy all names into the Name Picker for games.

https://docs.qq.com/sheet/DRUhDQ2hEVlNnQ1p5 (For Chinese users)

https://docs.google.com/spreadsheets/d/1-1hAMrEHT_vsWW4S8ENaJn5G5DbcugTr/edit#gid=252553682

Plenary and keynote abstract

Efficient Membranes for CO_2 Capture: Paths towards Industrial Applications

Academic, Liyuan Deng

Department of Chemical Engineering, Norwegian University of Science and Technology, Trondheim, Norway. *e-mail: liyuan.deng@ntnu.no

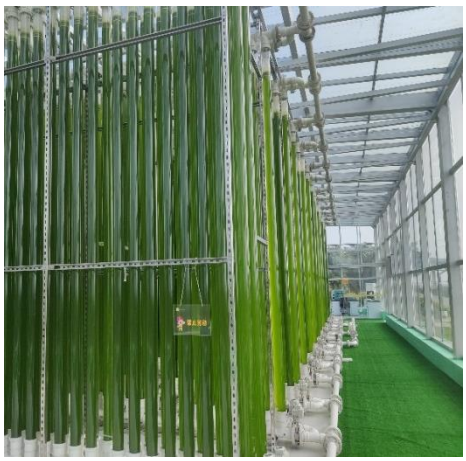
After decades of research and recent years' increasing interest in commercial development, membrane separation remains an "emerging" technology for industrial-scale carbon capture. Membrane materials with superior separation performance are undoubtedly the first requirement to make membrane-based CO_2 capture technology possible, but not the only one. In order for the membrane process to be feasible in an industrial process, the membrane should also have high stability under actual industrial conditions, with the possibility of making thin-film composite (TFC) membranes or membranes with thin skin layers in large-scale production.
NTNU's membrane research group has been working closely with industry to develop CO_2 separation membranes and, more recently, to capture CO_2 from various flue gases, such as from ships, platforms, and industrial processes. With industrial applications in mind, our strategy for developing viable membranes has been to 1) explore polymeric materials, including those not initially used for CO_2 separation; 2) enhance the facilitated transport mechanism of amine-based fixed site carrier (FSC) membranes, such as by optimizing membrane fabrication conditions, 3) introduce various efficient CO_2 mobile carriers, and 4) incorporate 0D to 2D nanofillers to enhance CO_2 transport. In this talk, several examples of how we have taken different approaches to improve various aspects of membrane properties for CO_2 capture will be presented, including optimization of polymer membrane matrices, studies on new mobile carriers, and the effects of embedding nanofillers.

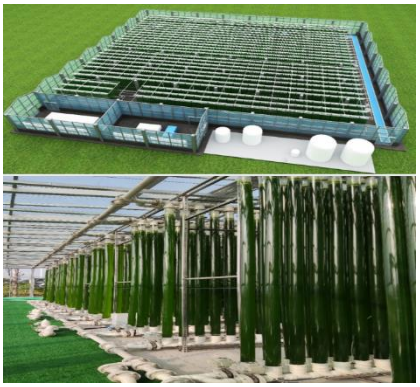
RESEARCH AND DEVELOPMENT OF CO_2 REDUCTION WITH MICROALGAE FROM COAL-FIRED FLUE GAS IN CHINA

Jun Cheng[1,2]*, Qiang Liao[1], Kefa Cen[2]

[1]Key Laboratory of Low-grade Energy Utilization Technologies and Systems of Ministry of Education, Chongqing University, 174 Shazheng Street, Chongqing 400044, China
[2]State Key Laboratory of Clean Energy Utilization, Zhejiang University, 38 Zheda Road, Hangzhou 310027, China
*e-mail:juncheng@zju.edu.cn

China has developed advanced microalgae technology with efficient photosynthesis reactions to utilize flue-gas CO_2 from coal-fired power plants and coal-chemical plants. Leading universities cooperated with pioneer companies have made breakthrough in developing cost-efficient photosynthetic reactors with robust microalgae species (*Spirulina*, *Chlorella* and *Nannochloropsis*). An industrial demonstration with an annual CO_2 fixation capacity of 10000 tons by microalgae has been built in erdos of Inner Mongolia. This project uses food-grade CO_2 with ≥99.95% concentration purified from coal chemical plants for cultivating *Spirulina* biomass. Another industrial demonstration with an annual CO_2 fixation capacity of 1000 tons by microalgae has been built in Yantai of Shandong Province. This project directly uses original flue-gas CO_2 with ~12% concentration from coal-fired power plants for cultivating *Nannochloropsis* biomass. Several central state-owned enterprises including China Resources Group and Guangdong Energy Group have largely invested in CO_2 reduction projects with microalgae from coal-fired flue-gas. The commercial operation of flue-gas CO_2 reduction with microalgae has been realized to sell microalgae biomass as nutritious food, functional feed and organic fertilizer. This brings significant environmental, social and economic benefits to green sustainable development.





CO_2 capture and conversion: Materials, Activity and Stability

C. Müller

Department of Mechanical and Process Engineering, ETH Zürich, Leonhardstrasse 21, 8092 Zürich, Switzerland. *e-mail:muelchri@ethz.ch

In this talk I will present recent advances in the development of effective and stable alkali earth metal oxide-based CO_2 sorbents and strategies to integrate them into catalytic processes. MgO and CaO-based CO_2 sorbents are promising materials owing to their (theoretically) high gravimetric CO_2 uptake capacity. However, deactivation due to sintering and poor kinetics (in the case of MgO) pose serious challenges with regards to their practical implementation. Here, I will describe our work aiming at elucidating the mechanisms that trigger deactivation, exploring approaches to accelerate the carbonation kinetics and present the development of strategies to stabilize the morphology of CaO-based CO_2 sorbents. The talk will be concluded by an example of integrating directly CO_2 capture into CO_2 conversion. Here, the CO_2 captured is directly converted into a synthesis gas (mixture of CO and H_2) using a Ni catalyst.

THE PHOTOCATALYTIC REDUCTION OF CARBON DIOXIDE – A MATERIALS OR A REACTOR ENGINEERING CHALLENGE?

Peter K. J. Robertson and Nathan Skillen

School of Chemistry and Chemical Engineering, Queen's University Belfast, David Keir Building, Stranmillis Road, Belfast, BT9 5GS.

The application of semiconductor photocatalysis for the reduction of carbon dioxide to practical fuel products such as methane, methanol or even two carbon products such as oxalate or glyoxalate, has been the subject of extensive research since the 1970s. The vast majority of this research has focussed on the development of new materials to enhance the yields of useful reduction products. Despite extensive work over the past four decades the overall yields of products tends to be in micromolar quantities per hour. In 2019, however, a significant step forward was reported with a copper oxide based material generating milli-molar quantities of methanol per hour.

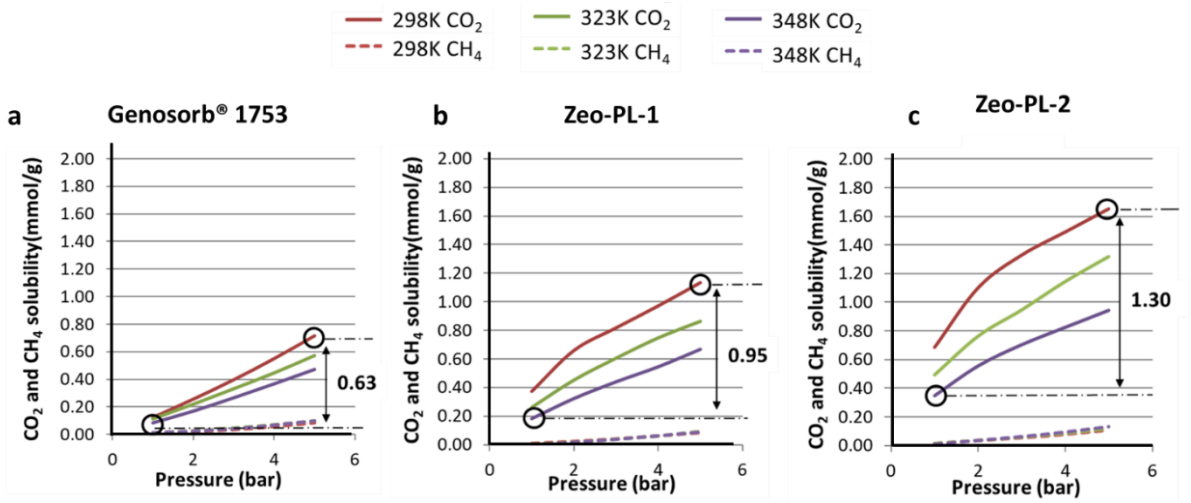
Despite this being an area of such active interest, there has been substantially less research into the engineering aspects of photocatalytic CO_2 reduction. For any practical system, even at prototype scale, it is going to be necessary to demonstrate the production of tens/hundreds of litres of cubic metre quantities of product. To achieve this, there are still big challenges with respect to both materials development and reactor engineering. The importance of reactor engineering has been previously demonstrated for other sustainable energy applications in photocatalysis such as water reduction or more recently biomass valorisation to generate hydrogen. In this presentation some of the key engineering challenges will be considered with respect to the background context of photocatalysis for sustainable energy production, with a focus on how lessons learned in other energy applications may be applied to the reduction of carbon dioxide.

POROUS LIQUIDS FOR CO_2 SEPARATION

S.L. James*

Queen's University Belfast, School of Chemistry and Chemical Engineering, Stranmillis Road, Belfast BT9 5AG. *e-mail:s.james@qub.ac.uk

Porous liquids are a new class of fluid absorbent with permanent well-defined, molecule-sized cavities [1-3]. Because of these cavities they exhibit very high gas uptakes and even size- or shape-selective gas uptake. We have been working on porous liquids with high CO_2 capacity and selectivity for applications in biogas upgrading, natural gas sweetening and ultimately post-combustion carbon capture. The porous liquids are dispersions of zeolites in commercial CO_2-capture poly-ether solvents such as Genosorb. They show 2-3 times the CO_2 uptake and CO_2/CH_4 selectivity of the commercial poly-ether solvents. Techno-economic analysis suggests that these porous liquids enable op-ex savings of 20-30%.



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2. N. O'Reilly et al. 2007, **13**, 3020.
3. J. Cahir et al. ***Chem. Sci.***, 2020,**11**, 2077-2084.

DEVELOPMENT OF FLUE GAS CO_2 CHEMICAL ABSORPTION TECHNOLOGY

M. Fang[1*], W. Dong[1], T. Wang[1], R. Zhao[2], D. Xu[2], Y. Wang[3], Q. Wang[1]

[1] Institute for Thermal Power Engineering, Zhejiang University, Hangzhou, P. R. China
[2] China National Energy Co., Ltd. Beijing, China
3 Guoneng Jinjie Energy Co., Ltd, Yulin, China
*E-mail: mxfang@zju.edu.cn

To realize carbon neutralization before 2060 is the national target of China. The carbon capture technology after combustion by chemical absorption method is considered to be the decarbonization technology with the most large-scale application prospect, which has attracted the attention of all countries. However, how to further reduce the investment cost and operation energy consumption of chemical absorption technology is the current research hotspot.

With the support of national key R & D projects of China, this paper aims at the key problems of chemical absorption technology. Firstly, this paper studies on the screening and performance evaluation of low-energy mixed amine absorbent and phase change absorbent. In view of the high cost of conventional stainless steel packing, hydrophilic modification of low-cost plastic packing is developed. A low-end differential all welded plate heat exchanger is developed for lean-rich solution heat exchanger. The heat exchange end differential temperature is less than 5 ℃. The performance of the new absorbent is tested on the 200Nm3/h chemical absorption pilot test platform. On this basis, a new type low-energy consumption process for chemical absorption of coal-fired flue gas, combined inter-stage cooling, rich liquid staged flow and MVR energy-saving process is put forward.

A 15Kt/a chemical absorption carbon capture demonstration project has been built and operated at Guoneng Jinjie Power Plant of Yulin in China. The system captured 15Kt/a CO_2 from coal fired flue gas for industrial utilization. While the flue gas volume rate is about 100,000NM3/h, inlet gas CO_2 concentration is about 12%, and optimal absorption liquid flow is about 340m3/h, the measured CO_2 regeneration energy consumption attains 2.75GJ/t CO_2, of which the capture rate is about 90%. When the inter-stage cooling, rich liquid staged flow and MVR energy-saving process were operated, the minimum regeneration energy consumption is about 2.278-2.378GJ/t CO_2. The operation cost of CO_2 capture is about US\$30/tCO_2 and total capture cost is about US\$40/tCO_2. It is expected to provide guidance for the industrial application of a new generation of carbon capture technology by chemical absorption.

Dual Function Materials, comprised of monolithic supported mixtures of catalyst and sorbent, for direct air capture of 400 ppm CO_2 in ambient air followed by catalytic methanation: The impact realistic condition

Robert J. Farrauto*, Chae Jeong, Potter, Monica Abdallah, Mark Goldman

Earth and Environmental Engineering,Columbia University in the City of New York 10027 USA.
Email: RF2182@Columbia.edu

A dual function material (DFM), comprised of Ru in intimate combination with a NaO supported on high surface area γ-Al_2O_3 is being investigated for direct air capture (DAC) of 400 ppm CO_2 followed methanation for production of renewable natural gas (CH_4). The process will be operated at ambient air conditions with waste or preferably green H_2 in a temperature swing mode. The data to be presented was generated using in simulated CO_2/air at ambient temperature and high humidity.

Experiments were conducted with DFM/Al_2O_3 granules with demonstrated stability in cyclic operation of CO_2 capture and conversion to RNG. Preliminary stability data on DFM washcoated ceramic monoliths will also be shown.

Our future reactor design will include deposition of the DFM on high cell density thin wall ceramic monoliths, typical of those used in the automotive catalytic converter. This design provides low pressure drop with suitable thin DFM/washcoat layers for high CO_2 capture allowing for rapid surface heating during temperature swing methanation.

The impact of humidity on different sorbents demonstrates the importance of laboratory evaluations under expected realistic DAC conditions.

Bob retired from BASF (formerly Engelhard), Iselin, NJ as a Vice President of Research in 2012. He immediately joined Columbia University, as a Professor of Professional Practice in the Earth and Environmental Engineering (EEE) Department.
He is the author (co-author) of 140 journal publications and 56 US patents. He is co-author of three catalyst textbooks, published by Wiley and Sons.
He is the recipient of a number of research awards.
He has a Google scholar rating of 54.

He received a BS from Manhattan College, Bronx, New York and PhD from Rensselaer Polytechnic Institute, Troy, New York.

Robert J. Farrauto, https://www.linkedin.com/in/robert-farrauto-18743618

CATALYST DEVELOPMENT FOR SUSTAINABLE FUEL & CHEMICAL PRODUCTION FROM CO_2

J. Huang[1,*]

[1] Laboratory for Catalysis Engineering, School of Chemical and Biomolecular Engineering, Sydney University, NSW 2006, Australia
*e-mail: jun.huang@sydney.edu.au

We are developing carbon capture methods that aim to go one step beyond storage, instead converting and recycling carbon dioxide (CO_2) into raw materials that can be used to create fuels and chemicals. We designed new catalysts for CO_2 hydrogenation to CH4 and CO in the current available reaction system. To simulate photosynthesis, we have built nanocatalyst microplates of carbon layered with carbon quantum dots with tiny pores that absorb CO_2 and water. Then a chemical process occurs on nanocatalysts that combines both compounds and turns them into hydrocarbon. Carbon dioxide is also an attractive feedstock for Carbon dioxide (dry) reforming of methane (DRM) is an attractive solution for the urgent Carbon Neutral Target since it involves not only the utilization of two greenhouse gases for sustainable production of market-favourite hydrogen and syngas, which can be achieved on the large scale using the existing infrastructure. Ni-based catalysts with high activity are promising in commercial DRM process, however, they suffer from quick deactivation due to the lack of knowledge regarding the surface composition and geometry under working conditions. In the present study, we applied *in situ* high resolution transmission electron microscope (HRETEM) coupled with mass spectroscopy (MS) in one working platform for monitoring both the catalyst dynamic and geometry with the reaction mechanisms occurring under working conditions for DRM on Ni catalysts. We provide evidence for each reaction pathway associated with the property of surface active sites. This research focuses on providing insight into the reaction and deactivation mechanisms of Ni catalysts in the DRM, but the obtained knowledge is significant also for the investigation of many catalysis challenges both in research and engineering.

Biomass Pyrolysis for Biochar and Its High-value Utilization

Haiping Yang, Yingquan Chen, Mingwei Xia, Sunwen Xia, Wei Chen, Hanping Chen

State Key Laboratory of Coal Combustion, School of Power and Energy Engineering, Huazhong University of Science and Technology, 430074 Wuhan, China

Email: yhping2002@163.com

Biochar as a platform carbon material, through modification and functionalization for high-value and high-performance carbon materials, is becoming a hot utilization direction of biomass. Pore structure and highly active functional groups are two main factors for the energy storage and CO_2 adsorption. exogenous nitrogen (NH_3, etc.) was introduced during biomass pyrolysis and activation to further enhance the adsorption and electrochemical performance of biochar materials. The specific surface area of N-doped biochar product reached 2417 m^2/g with ~4 wt.% nitrogen content, and small mesoporous proportion was as high as 98%, and the specific capacitance can reach 323.3 F/g. A new method for preparation of high-value N-doped porous biochar materials was formed. Also for the green activation, activation mechanism of CH_3COOK, presenting non-toxic, low corrosive, and developed a green preparation method for nano porous biochar materials with high specific surface area. The melting, decomposition and crystallization before 700℃ made the porous biochar product present a certain piece of laminar morphology with the thickness of about 60 nm, and the specific surface area can reach 1500 m^2/g. Graphitization degree of biochar material is also an important index of carbon materials. Mesoporous biochar graphite materials from biomass was prepared, and the role of iron in pyrolysis process was explored. It realized graphitization degree (40-100%) temperature and iron load regualtion.

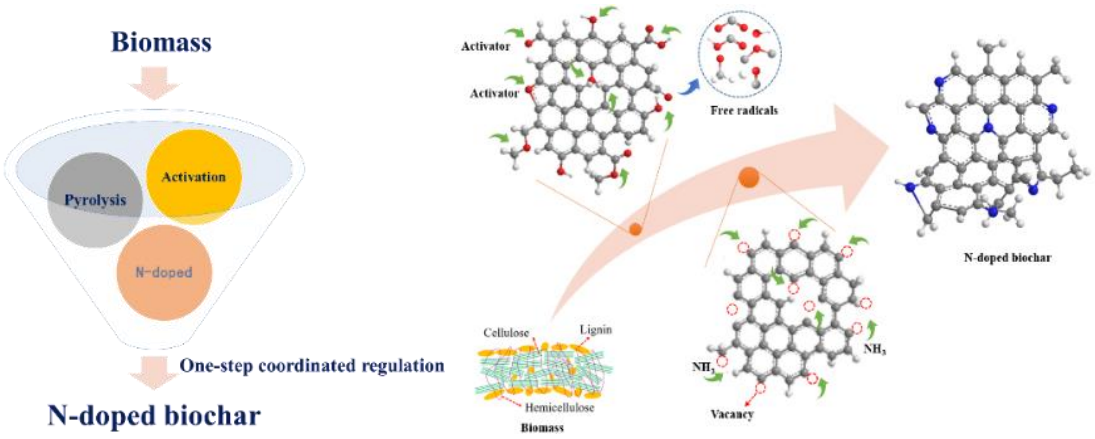


Figure 1. Biomass pyrolysis for high-value biochar materials

Systems Engineering for Carbon Capture and Utilisation in the context of CCUS

Meihong Wang*

Department of Chemical and Biological Engineering, the University of Sheffield, UK
*e-mail:Meihong.Wang@sheffield.ac.uk

The talk will start with an introduction to Systems Engineering, followed by motivations of our research. The main part will be our research on carbon capture and transport in the context of Carbon Capture, Utilisation and Storage (CCUS) for Power Plants. Then the topic will be extended to our current efforts in CCUS for petro-chemical manufacturing (e.g. ethylene plants). In the end, we will also discuss how to apply Artificial Intelligence techniques for modelling, optimisation and control in CCUS.

Pretreatment and hydrolysis of lignocellulosic Biomass for Biorefineries

Zhen Fang
Academic, Editor-in-Chief, Springer Book Series - Biofuels and Biorefineries
Fellow of the Canadian Academy of Engineering,
Associate Editor of J Renew Mater, Biotechnol Biofuels, and J Supercrit Fluid
Biomass Group, College of Engineering, Nanjing Agricultural University
40 Dianjiangtai Road, 210031 Nanjing, Jiangsu, China
email: zhenfang@njau.edu.cn
URL: ORCID iD: http://orcid.org/0000-0002-7391-372X; https://biomass-group.njau.edu.cn/

This presentation covers three parts: pretreatment and hydrolysis of lignocelluloses (enzymatic, catalytic and fast hydrolyses), biodiesel production, and synthesis of chemicals and biofuels.

First, for hydrolysis, (i) Pretreatment techniques for enzymatic hydrolysis at lower temperature (50 °C) were studied. Organic electrolyte solution composed of ionic liquid and organic solvent {i.e., [AMIM]Cl) + DMSO}, was prepared and used for the treatment of cellulose and wood for their subsequent enzymatic hydrolysis. Other organic solvents (e.g., acetone-water, diol, glycerol, ethylene glycol), ball-milling and fungi pretreatment techniques are also covered. (ii) For catalytic hydrolysis, some heterogeneous catalysts with nano- or micro size were synthesized by co-precipitation and calcination in order to hydrolyze biomass at mild temperature (e.g., 180 °C). Activated hydrotalcite nanoparticles, calcium ferrite and magnetic carbonaceous sulfonated acid catalyzed the hydrolysis of biomass with high glucose yield. These catalysts can be easily recovered for recycles. (iii) Fast hydrolysis process is introduced. By adding 0.8 wt% Na_2CO_3 in water, wood without any pretreatment can be completely dissolved upon fast-heating (7~16 °C/s) to form a 'wood solution' at 329–367 °C over short reaction times (0.7–2 s). The 'wood solution' is rapidly (approximately 15 s) hydrolyzed to sugars/sugar oligomers under homogeneous conditions. Based on this finding, a 'fast hydrolysis' process was invented for actual lignocellulosic biomass in a flow reactor to produce sugars.

Secondly, a green process was developed for the production of biodiesel using magnetic solid catalysts instead of conventional liquid catalysts that are unrecoverable. The solid catalysts can be easily separated magnetically for recycles and successfully used for Jatropha biodiesel production. Microwave and ultrasound techniques were also introduced to promote biodiesel production.

Finally, nanocatalysts were synthesized to catalyze the high yield production of liquid biofuels (e.g., methyl levulinate, γ-valerolactone, 2,5-dimethylfuran, methylfuran) at low temperatures directly from carbohydrates (e.g., sugars, cellulose). It is found that 95% 2,5-dimethylfuran yield was obtained from fructose at 110 °C, 99% 2,5-dimethylfuran yield from 5-hydroxymethylfurfural and 97% 2-methylfuran yield from furfural were even achieved at room temperature (25 °C) when polymethylhydrosiloxane was used as H-donor. Therefore, liquid biofuels (e.g., 2,5-dimethylfuran) can be produced from sugars via the hydrolysis of lignocellulosic biomass that is easy for commercial applications in simple and inexpensive reactors.

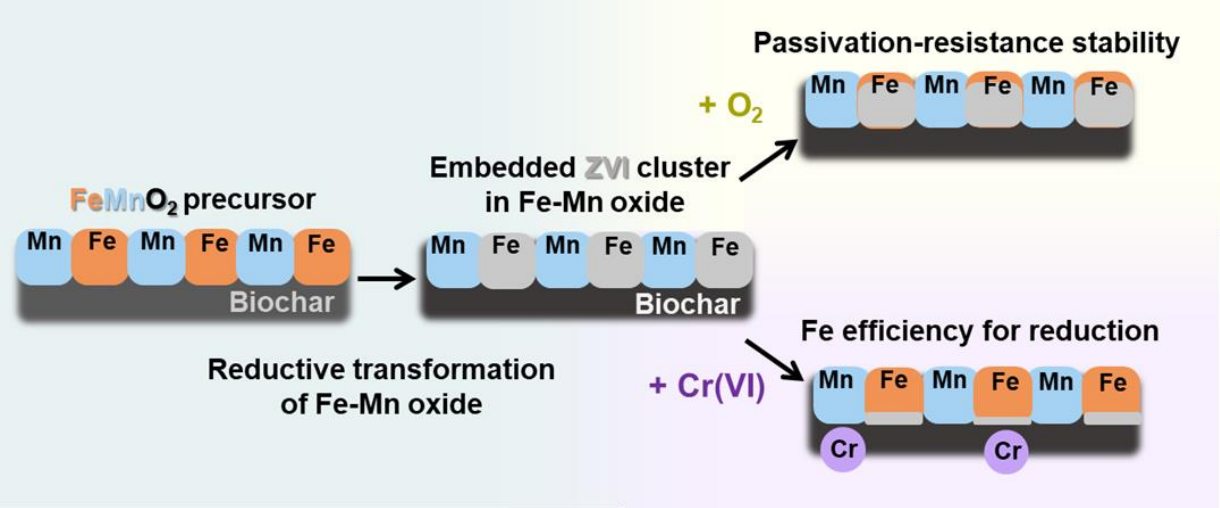
Keywords: Pretreatment; Hydrolysis; Biodiesel; Liquid fuels; Nanocatalysts

Customized Design of Iron-Manganese Oxide Clusters on Biochar Composites

Zibo Xu and **Daniel C.W. Tsang***

Department of Civil and Environmental Engineering, The Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong, China
*e-mail:dan.tsang@polyu.edu.hk

The dense surface passivation layer on zero-valent iron (ZVI) restricts its practical application for reduction-determined processes, while fabrication of ZVI-based material with passivation-resistance stability is still challenging. Herein, we distribute Fe-Mn oxide precursor on biochar with pyrolysis for the customized formation of embedded ZVI clusters in the Fe-Mn oxides, which could exhibite higher electron-donating efficiency and passivation-resistance stability than the ZVI alone. The oxygen atoms in the FeO structure were removed during the pyrolysis, while the MnO skeleton in $FeMnO_2$ was preserved, resulting in the formation of embedded ZVI clusters. A potent efficiency for reducing Cr(VI) was observed in the embedded ZVI clusters compared with ZVI alone because the formed Cr(III) did not form the Fe-Cr passivation shell in the presence of Mn structures. More importantly, higher oxidation-resistance stability was found in the embedded ZVI clusters than in ZVI alone, with a lower decrease in the Cr(VI) removal performance after natural or accelerated oxidation. $FeMnO_2$ was formed during the oxidation of the embedded ZVI clusters, and the surface coverage inhibited the diffusion of Fe in the oxide layer and its interaction with O_2. Further oxidation of the embedded ZVI clusters was hampered with a thinner Fe oxidation layer (~20−50 nm) than the ZVI alone (~100 nm). Our study sheds light on the binary oxide transformation on biochar composites and provides a new approach to develop active ZVI-based materials with high Fe efficiency and stability.


Passivation-resistance stability
+ O_2
Mn Fe Mn Fe Mn Fe
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in Fe-Mn oxide
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Biochar
Fe efficiency for reduction
Reductive transformation
of Fe-Mn oxide
+ Cr(VI)
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Cr

Ocean Carbon Capture Using Membrane Contactors

Katherine Hornbostel

University of Pittsburgh

*e-mail:hornbostel@pitt.edu

Negative emissions technologies are needed at a Giga-ton scale by 2050 in order to keep global temperature rise below the 1.5°C threshold. Although plenty of research has gone into direct air capture technology, very little research has been done on direct ocean capture (DOC). Whereas direct air capture suffers from large system sizes and high energy costs to blow large volumes of air through the system, DOC could be more compact and require less energy due to the higher CO_2 concentration per unit volume. Furthermore, a large-scale DOC system could have the added benefit of controlling local ocean pH in a high-risk marine environment such as a coral reef or shellfishery. A couple of research teams have investigated electrochemical DOC approaches, but these processes require exorbitant energy inputs to separate seawater into acidic and basic streams before stripping CO_2. Our team is proposing a fundamentally different DOC approach that involves flowing seawater through a membrane contactor, where CO_2 diffuses through the membrane and reacts with NaOH solvent on the other side. This kind of technology has been successfully implemented in traditional carbon capture applications and is a promising fit for DOC due to low energy costs, compact/efficient separation, and the benign NaOH solvent. Our team is researching two design configurations for this technology (as shown in the attached figure): hollow fiber membranes and encapsulated solvents. We have developed 1D models for each design, and the results from these models demonstrate reasonable breakthrough times and CO_2 fluxes. We have also performed bench-scale experiments for each design that demonstrate CO_2 flux from synthetic seawater into the solvent. Finally, we have performed preliminary techno-economic calculations to estimate the size, cost and energy penalty of DOC using these two types of membrane contactors. Together these results demonstrate the potential for this novel negative emissions technology.

Polymeric membranes for CO_2 capture: from lab to industry

Jing Wei[1,2,3,4], Yulei Ma[1,2,3,4], Hongfang Guo[1,2,3,4], Zikang Qing[1,2,3,4], Jianan Fan[1,2,3,4], Zhongde Dai[1,2,3,4*]

1College of Architecture and Environment, Sichuan University, Chengdu 610065, China

2National Engineering Research Centre for Flue Gas Desulfurization, Chengdu 610065, China

3Carbon Neutral Technology Innovation Center of Sichuan, Chengdu 610065, China

4School of Carbon Neutrality Future Technology, Sichuan University, Chengdu 610065, China

*e-mail: zhongde.dai@scu.edu.cn

Polymeric membranes are gaining increasing attention for CO_2 capture. Despite the significant progress in the recent decades, the trade-off between gas permeability and selectivity in polymeric membranes has limited the large scale application of membrane technology. Developing membrane materials with both high gas permeability and selectivity is critical to make membrane gas separation processes more competitive compared to the current commercial separation technologies.on the othe hand, fabricating thin film composite (TFC) membranes with proper CO_2 flux and fabricating membrane modules which could fullfill requirent of industrial applications is another critical step in membrane based CO_2 capture.

In the past few years, lots of efforts have been devoted to high performance CO_2 membrane materials developement as well as TFC membrane/membrane module fabircation. Facilitated membranes, Mixed matrix membranes with bio-based nanofillers, as well as molecular rearranged memrbanes have been developed. In addition, some membrane mateirals have been fabricated into TFC membranes, and membrane modules with membrane area of over 10 m^2 have been developed.

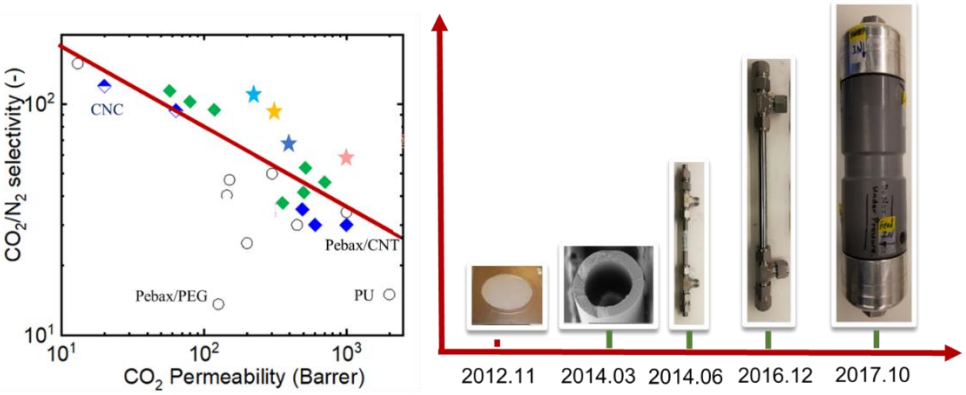


Figure 1. Membrane mateirals developed and membrane module development

SUSTAINABLE CO_2 CAPTURE VIA ADSORPTION BY CHITOSAN-BASED FUNCTIONAL BIOMATERIAL DERIVED FROM BIOREFINERY APPLICATION: A REVIEW ON RECENT ADVANCES, CHALLENGES, AND FUTURE PROSPECTS

Su Shiung Lam[1,*], Shin Ying Foong[1], Yi Herng Chan[2], Peter Nai Yuh Yek[3], Pock Keey Liew[4]

[1] Pyrolysis Technology Research Group, Institute of Tropical Aquaculture and Fisheries (AKUATROP), Universiti Malaysia Terengganu, 21030 Kuala Nerus, Terengganu, Malaysia.
[2] PETRONAS Research Sdn. Bhd. (PRSB), Lot 3288 & 3289, off Jalan Ayer Itam, Kawasan Institusi Bangi, 43000 Kajang, Selangor, Malaysia.
[3] Centre for Research of Innovation and Sustainable Development, University of Technology Sarawak, No.1, Jalan Universiti, Sibu, Sarawak, Malaysia.
[4] NV Western PLT, 208B, Macalister Road, 10400 Georgetown, Penang, Malaysia.
*e-mail:lam@umt.edu.my ; sushiung@gmail.com

Chitin is a naturally occurring biopolymer that is present in abundance in biomass after cellulose, while chitosan is the deacetylated-derivative of chitin that can be obtained as a value-added functional biomaterial from biorefinery application. Its unique properties such as biodegradability, non-toxicity, high adsorption capacity and biocompatibility allows them to be utilized as adsorbent for CO_2 capture. The present review provides a detailed and specific overview of chitosan-based functional biomaterial derived from biorefinery of biomass as adsorbent for CO_2 capture. Various extraction methods of chitin/chitosan from biomass are discussed and compared (including chemical, biological, green solvents, microwave, ultrasonic, supercritical fluid, and hybrid treatment), followed by the discussion of synthesis techniques of chitosan-based adsorbents for CO_2 capture (including carbonization, pyrolysis, chemical activation, and chemical modification/impregnation). The structural characteristics of chitosan-based adsorbents and the effect of process parameters of CO_2 adsorption are reviewed to highlight the potential of chitosan-based adsorbent in CO_2 capture. Furthermore, the technological gaps and limitations of each extraction and synthesis techniques are elucidated, as well as the overall challenges and outlook of the subject matter.

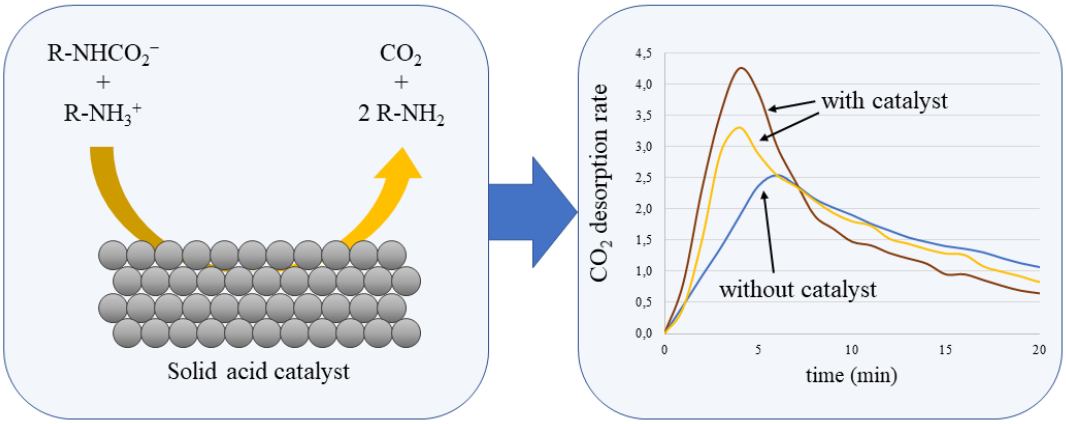
Keywords: chitin; chitosan; extraction; adsorbent synthesis; CO_2 capture

INNOVATIVE CO_2 CAPTURE PROCESSES BASED ON NONAQUEOUS AMINE SORBENTS AND SOLID ACID CATALYSTS FOR LOW-TEMPERATURE REGENERATION

F. Barzagli[1,*], A. Ienco[1], M. Peruzzini[1] and U.H. Bhatti[2]

[1] National Research Council of Italy (CNR), ICCOM Institute, Via Madonna del Piano 10, 50019 Sesto Fiorentino, Florence, Italy
[2] KAUST Catalysis Center (KCC), King Abdullah University of Science and Technology, Thuwal 23955, Saudi Arabia
*e-mail: francesco.barzagli@iccom.cnr.it

Chemical capture of carbon dioxide (CO_2) from industrial flue gases by aqueous amine solutions is considered one of the most mature and effective techniques to lower CO_2 emissions into the atmosphere, and its rapid development is deemed crucial to curb global warming and related climate change. Unfortunately, the high energy cost of sorbent regeneration has so far greatly limited the industrial application of this technology. Aiming at lowering the energy demand for desorption, several strategies have recently been developed: among them, two of the most interesting involve the use of solid acid catalysts in the desorption process, to promote the regeneration of the aqueous sorbent at lower temperatures, or even the replacement of water with organic diluents, thus formulating nonaqueous amine sorbents in which the organic diluent has a significantly lower heat capacity than water and the products formed during absorption are more easily degraded. In order to develop an innovative CO_2 capture approach potentially capable of significantly reducing the energy required for the entire process, we decided to combine these two strategies together, using nonaqueous sorbents in the presence of solid acid catalysts to increase desorption kinetics. Stable alkanolamine 2-(2-aminoethoxy)ethanol (DGA) was dissolved in two different organic diluents, namely diethylene-glycol-monomethyl-ether (DEGMME) and a 1:1 mixture of ethylene glycol and 1-propanol (EG/PrOH), and the resulting solutions were used to efficiently capture CO_2 from a gas stream. Next, their regeneration performance was evaluated with and without some solid acid catalysts, already proved to work with aqueous sorbents. In addition, the desorption mechanisms were investigated through ^{13}C-NMR speciation analysis. As a preliminary result, we found that some metal oxide can effectively catalyze the carbamate breakdown and the subsequent CO_2 release, thus reducing the total heat requirement.

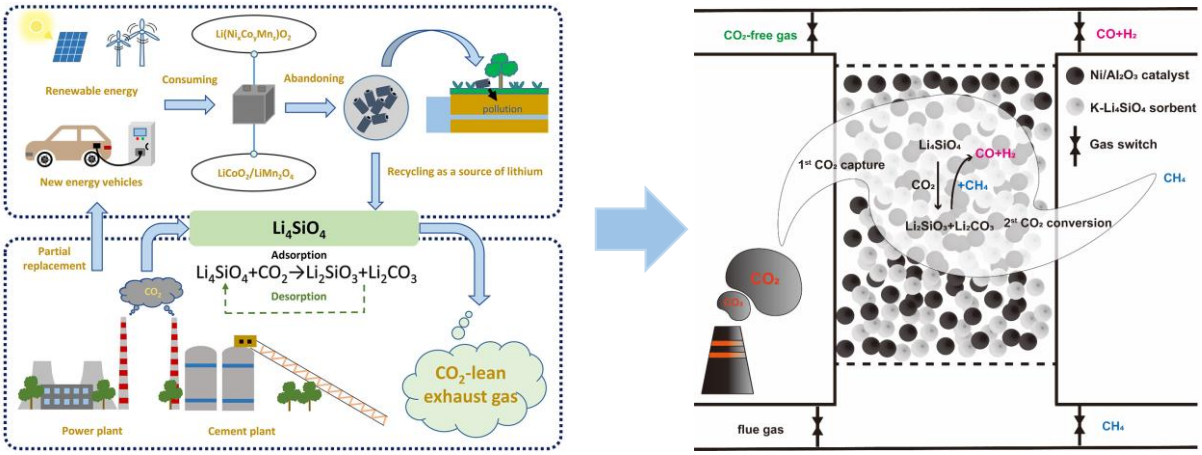

R-NHCO2−
+
R-NH3+
CO2
+
2 R-NH2
Solid acid catalyst
CO2 desorption rate
4,5
4,0
3,5
3,0
2,5
2,0
1,5
1,0
0,5
0,0
0
5
10
15
20
time (min)
with catalyst
without catalyst

Construction of Efficient and Low-Cost Li_4SiO_4 and the Integrated CO_2 Capture/Conversion by DRM

Changlei QIN

Key Laboratory of Low-grade Energy Utilization Technologies and Systems of Ministry of Education, School of Energy and Power Engineering, Chongqing University, Chongqing 400044, China
*e-mail:c.qin@cqu.edu.cn

Comparing with the conventional step-by-step CO_2 capture and utilization, the integrated CO_2 capture and conversion (ICCC) can simplify the process flow and reduce energy consumption. The realization of ICCC largely depends on the matching features of CO_2 adsorption/catalytic materials. In particular, sorbents run through the whole process of CO_2 capture and the sequential in-situ conversion, playing a key role in the technology. Herein, the development of high-performance Li_4SiO_4 and its application in ICCC would be presented. First, Li_4SiO_4 particles with excellent adsorption and mechanical properties were prepared by an extrusion-spheronization method. The optimized particles can not only achieve a stable CO_2 capacity of 0.31 g/g, but also have a compressive strength of 27.5 MPa. Then, a route in synthesizing low-cost Li_4SiO_4 from spent lithium-ion batteries (LIBs) was proposed. Performance evaluation show that Li_4SiO_4 synthesized from the cathode of LIBs has superior CO_2 capture characteristics (around 0.19 g/g under 15 vol.% CO_2 after 80 cycles), and the synthesis cost from LIBs is only 1/20-1/3 of the conventional methods. Moreover, basic reaction characteristics of ICCC-DRM adopting Li_4SiO_4 were investigated. It is found that the H_2/CO output ratio is stablized at 1±0.05 and the duration is prolonged with increasing cycle number, showing good process matching and stability. These results can provide useful reference for the development of integrated CO_2 capture and conversion technology.

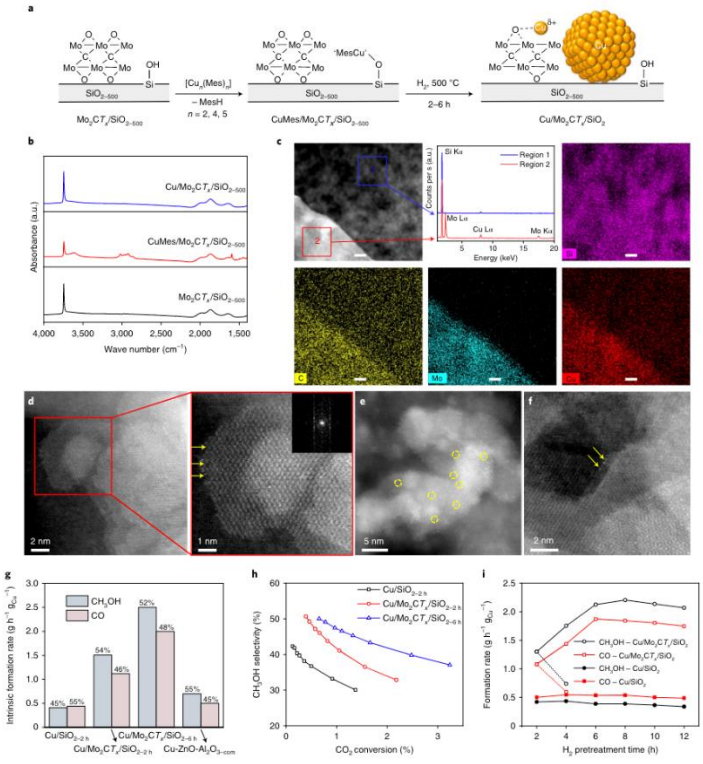


2D molybdenum carbide (MXene) for CO_2 hydrogenation

Hui Zhou*

Department of Energy and Power Engineering, Tsinghua University, Beijing 100084, China
*e-mail:huizhou@tsinghua.edu.cn

Currently, the conversion of captured CO_2 into value-added chemicals or fuels is considered a key strategy to mitigate the yet increasing anthropogenic CO_2 emissions, in particular when combined with H_2 obtained using renewable energy. Depending on the catalyst and the reaction conditions used, thermocatalytic CO_2 hydrogenation can give CO, methanol, dimethyl ether (DME), methane, or heavier hydrocarbons. MXene materials, that is, a family of two-dimensional (2D) carbides, nitrides and carbonitrides with the general formula of $M_{n+1}X_nT_x$ (where M is an early transition metal, n = 1, 2, 3, X is C and/or N and *T* are surface –O–, –OH and/or –F groups), are currently emerging in thermocatalytic applications as catalysts or supports with reactive metal–support interactions. Enabled by the scalable synthesis of MXenes, we report a gram-scale synthesis of a phase-pure multilayered hexagonal 2D-Mo_2C material with only Mo-terminated basal planes. 2D-Mo_2C is by a factor of six per mass of catalyst more active for CO formation than the reference β-Mo2C catalyst and shows no deactivation on stream for more than 100 h. We also report that silica-supported, dispersed, reducible nanosheets of a delaminated molybdenum MXene, Mo_2CT_x, can be used to engineer a Cu/Mo_2CT_x interface that shows an at least six times increased intrinsic formation rate of methanol by the direct hydrogenation of CO_2 compared to Cu/SiO_2.



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Invited abstract

Hydrothermal conversion of pectin under a temperature-pressure independent process

Hydrothermal conversion can convert biomass into carbon materials in catalysis, energy storage, and water purification. Pectin, a polysaccharide widely presented in plant cell walls, is an important component of biomass. However, the formation and evolution of pectin-derived hydrothermal carbon are not clear. In this study, we conducted the hydrothermal treatment of pectin at 100–300 °C to investigate the properties at different hydrothermal stages. With the characterization of the solid products with scanning electron microscopy (SEM), elemental analysis, N_2 adsorption/desorption, Fourier-transform infrared (FTIR) spectroscopy, Raman spectroscopy, X-ray photoelectron spectroscopy (XPS), and pyrolysis behavior in thermogravimetric analyzer (TGA), we proposed the formation and evolution pathway of pectin-derived hydrothermal carbon from original pectin. Pectin first underwent a physical change of gelation during the hydrothermal process, and then was hydrolyzed to liquid monomers. Pectin-derived hydrothermal carbon was formed by the polymerization of liquid monomers resulting from the hydrolysis of pectin. Moreover, the hydrothermal carbon was further carbonized, accompanied by dehydration and aromatization. Meanwhile, the originally irregular pectin bulk structure was completely transformed into carbon spheres above 200 °C. This work can provide some fundamental guidance for the sustainable synthesis of carbon materials from the hydrothermal process of pectin.

A novel supercritical CO_2 based natural gas fuelled power cycle for ultrahigh efficiency energy generation with inherent carbon capture

Syed Saqline [a], Alessandro Romagnoli [b*], Wen Liu [a*]

a. School of Chemical and Biomedical Engineering, Nanyang Technological University, 637459, Singapore

b. School of Mechanical and Aerospace Engineering, Nanyang Technological University, 639798, Singapore

The Allam cycle is a class of oxy-fuel combustion power cycles using supercritical CO_2 as the thermal fluid for power generation, with inherent capture of CO_2. Compared to other conventional CO_2 capture techniques, the Allam cycle stands out because of its high fuel-to-electricity conversion efficiency, elimination of the need for steam Rankine cycle and reduced physical footprint. A key source of energy penalty of Allam cycle comes from the cryogenic air separation unit (ASU), which supplies pure oxygen to the natural gas combustion process. This paper presents a thermodynamic analysis of a novel supercritical CO_2 -based power generation scheme, in which a natural gas fuelled Allam cycle is integrated and supported by a chemical looping air separation (CLAS), which supplies oxygen to the combustor with reduced energy consumption. The modelling results show that the Allam-chemical looping air separation (Allam-CLAS) process can achieve 54.6% net electrical efficiency with close to 100% CO_2 capture rate. This is higher than the traditional Allam cycle coupled to a cryogenic ASU. This newly proposed Allam-CLAS power cycle is a zero-carbon, highly efficient, and cost-competitive solution for decarbonising natural gas-fuelled electricity.

Rheology of Portland Cement Blended with Synthetic Calcium Carbonate from Mineral Carbon Capture and Utilization

Eleni Vlachou, Rukayat Salawu, Lewis J. McDonald, Yeshui Zhang, Waheed Afzal*

School of Engineering, University of Aberdeen, Aberdeen, United Kingdom, AB24 3UE

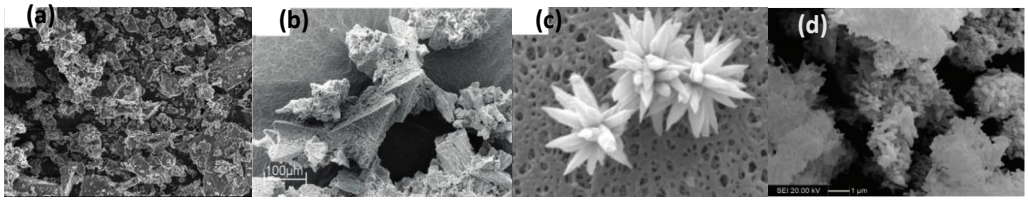
* Corresponding author: waheed@abdn.ac.uk

Abstract

Cement manufacturing accounts for 6-7% of industrial carbon dioxide emissions globally. In other to mitigate the emissions, we propose addition of carbon-negative precipitated calcium carbonate ($CaCO_3$) obtained from carbon capture from flue gas as supplementary cementitious material using mineral Carbon Capture and Utilization (CCU) strategies. Our earlier results show that the addition of synthetic calcium carbonate, when in the right purity and morphology, can increase the compressive strengths at 7-day and 28-day hydration. However, the compressive strength is not the only engineering property of interest for the full-scale adoption of cement blends as a construction building material.

This study examines the rheological properties of cement blends with additives (different types of calcium carbonate) in different ratios and quantities. Nano-calcite aragonite in powder form and scalenohedral calcium carbonate in crystalline form are added in Portland cement at mass parentage from 5% to 15% and water/solids ratio varying from 0.47 to 0.53 (W:S). Ordinary Portland cement CEM I 52.5N is used in all experiments whereas three different types of calcium carbonate are used in all experiments. To study the workability of cement-blend pastes, different rheological properties are measured to calculate yield stress (τ_y), the plastic viscosity (μ_p) and the apparent viscosity to establish types of non-Newtonian behavior.

Based on our experimental results from this work and those from an ongoing project, we can demonstrate that the addition of carbon-negative synthetic calcium carbonate solids can influence several engineering properties of hydrated cements in terms of strength, workability and early strengths offering avenues to reduce carbon footprint of cement manufacturing.



Scanning-electron microscopes of different morphological types of $CaCO_3$.
(a) ground, **(b)** scalenohedral, **(c)** aragonite, **(d)** nano-calcite

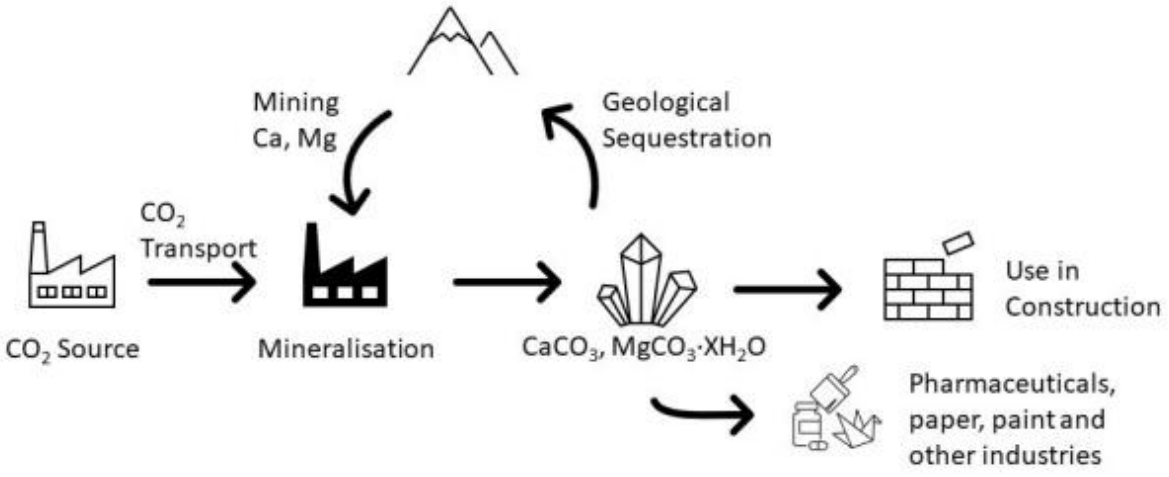
Mineral Carbonation for Industrial Decarbonisation of Portland Cement and Additives

Lewis J McDonald[1,2*], Eleni Vlachou[1], Wanawan Pragot[1,3] and Waheed Afzal[1]

[1] School of Engineering, University of Aberdeen, Aberdeen, United Kingdom, AB24 3UE
[2] Dept. of Mechanical Engineering, University of Bath, Bath, United Kingdom, BA2 7AY
[3] University of Phayao, Amphur Muang Phayao, 56000, Thailand
*e-mail:ljm222@bath.ac.uk

The use of carbon capture technologies has been put forward by the International Energy Agency (IEA) as the preferred solution to utilise carbon dioxide from Portland cement production. Production of Portland cement emits CO_2 in the range of 0.85 to 0.95 kgCO_2-eq/kg cement using current technologies. Clinker, the major ingredient of cement accounts for 90% of carbon dioxide emissions in cement production; during clinker production, 50% of the carbon dioxide is produced during the calcination of raw materials and 40% carbon dioxide is produced from the combustion of fuels to produce sufficient thermal energy to heat rotary kilns which account. About 10% carbon dioxide is produced from the raw material and clinker size reduction, transportation and distribution.

Implementation of mineral carbon capture and utilisation (MCCU) to rotary cement kilns and fuel source gives rise to the potential for the cement industry to produce useful mineral carbonates including calcium and magnesium carbonates. These minerals are used in several industries as well as have the potential to create a circular cement economy. Through conducting a cradle-to-gate life cycle analysis of calcium carbonate produced by MCCU, it has been determined that CO_2 from Portland cement production can be reduced by up to 67%. The MCCU process used in this research captures the CO_2 through reacting it with an alkali, NaOH, and uses aqueous metal ions to precipitate metal carbonates. The life cycle impact assessment aided in identifying improvement potentials for the MCCU process to potentially further reduce CO_2. Furthermore, the $CaCO_3$ precipitated was added to Portland cement as a supplementary cementitious material, improving on key engineering properties including setting time, compressive strength and rate of hydration.


Mining
Ca, Mg
Geological
Sequestration
CO_2
Transport
Use in
Construction
CO_2 Source
Mineralisation
$CaCO_3$, $MgCO_3 \cdot XH_2O$
Pharmaceuticals,
paper, paint and
other industries

Development of Cryogenic CO_2 capture technologies

C. Song [1,*], Q. Liu [1], S. Deng [1], H. Li [2] and Y. Kitamura [3]

[1] Tianjin Key Laboratory of Indoor Air Environmental Quality Control, School of Environmental Science and Technology, Tianjin University, 92 Weijin Road, Nankai District, Tianjin, P.R. China

[2] Mälardalen University, School of Sustainable Development of Society and Technology, SE-721 23 Västerås, Sweden

[3] Graduate School of Life and Environmental Sciences, University of Tsukuba, 1-1-1, Tennodai, Tsukuba, Ibaraki 305-8572, Japan

*e-mail:chunfeng.song@tju.edu.cn

CO_2 capture, utilization and storage (CCUS) have been recognized as the primary option to mitigate the issue of climate change caused by the utilization of fossil fuels. In last decades, several CO_2 capture approaches have been developed, such as absorption, adsorption, membrane, chemical looping, hydrate and biofixation etc. Among different technologies, a particularly attention has been paid on cryogenic CO_2 capture by phase change. The aim of this study is to develop an interest in cryogenic technologies for CO_2 capture based on an overview of the actual situation of CCS. To reach this aim, the major CO_2 capture strategies and technologies from fossil fuel combustion has been reviewed. Simultaneously, the characteristics of cryogenic technologies for CO_2 capture are summarized. The existing challenges with the need to overcome for cryogenic technology include cold energy sources, capture cost and impurities, etc. Finally, the opportunities of the future development for cryogenic based technologies are discussed. The investigation results indicated that cryogenic CO_2 capture processes can be easily retrofitted to the existing industrial emission facilities, and avoids the challenges associated with chemical solvents or physical sorbents.

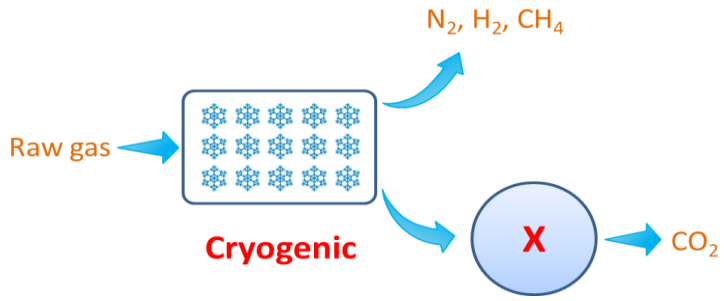


Fig.1 Cryogenic standalone and its based hybrid CO_2 capture strategy

Molecularly engineering polybenzimidazole for efficient pre-combustion CO_2 capture

Leiqing Hu, Haiqing Lin*

Department of Chemical and Biological Engineering, University at Buffalo, The State University of New York, Buffalo, NY, 14260, USA
*e-mail:haiqingl@buffalo.edu

Membrane materials with superior H_2/CO_2 separation properties at high temperatures are of great importance for pre-combustion CO_2 capture. Conventional material designs often focus on rigid polymers with strong size sieving ability to enhance H_2/CO_2 diffusivity selectivity, which, however, often lowers gas permeability, limiting its competitiveness over other separation technologies. To circumvent this conundrum, we have designed polymer architectures comprising bottlenecks to enhance the size-sieving ability and microcavities to increase gas diffusivity. We start from polybenzimidazole (PBI), one of the leading polymers for H_2/CO_2 separation with H_2 permeability of 27 Barrer and H_2/CO_2 selectivity of 16 at 150 °C. PBI also contains imidazole rings that offer great versatility for molecular engineering. First, PBI can be doped with thermolabile cross-linkers before low-temperature carbonization to retain the polymer processability and achieve superior H_2/CO_2 separation properties. Specifically, PBI is cross-linked with pyrophosphoric acid (PPA) via H-bonding and proton transfer to create sub-3.3 Å ultramicropores before carbonization at <600 °C. PPA degrades at ≈ 200 °C, much lower than PBI (≈580 °C), creating microcavities during carbonization. The PPA doping and pyrolysis increase H_2 permeability to 140 Barrer and H_2/CO_2 selectivity to 58, above Robeson's upper bound at 150 °C. Moreover, when challenged with simulated syngas containing water vapor, the obtained membranes demonstrate stable mixed-gas selectivity for 105 h. Second, I will describe the in-situ synergistic growth of **c**rystalline zeolite imidazole framework-8 (ZIF-8) and **p**olymer-incorporated **a**ZIF-8 **m**ixed matrix materials (CPAMs). The formed porous crystalline ZIF-8 (cZIF-8) acting as microcavities, increases gas permeability. More importantly, the imidazole rings in PBI induces the formation of amorphous ZIF-8, enhancing size-sieving ability. For example, the formation of 15 mass% ZIF-8 in PBI improves H_2 permeability and H_2/CO_2 selectivity by ≈100% at 35 °C. The CPAM shows stable H_2/CO_2 separation performance (H_2 permeability of 42 Barrer and H_2/CO_2 selectivity of 28) at 200 °C, surpassing the Robeson upper bound. The structure/property relationships in these two series of polymers will be elucidated to demonstrate that the creation of dual free volumes can effectively break the permeability/selectivity tradeoff for membrane gas separations.

PLASMA-ENABLED FAST LIQUEFACTION OF LIGNOCELLULOSIC BIOMASS

D.H. Mei *, S.Y. Liu, S. Wang, Z. Fang

College of Electrical Engineering and Control Science, Nanjing Tech University, Nanjing 211816, Jiangsu China
*e-mail:danhuam@126.com

Biomass is one renewable carbon-containing energy resource. The effective use of biomass energy can meet the requirements of carbon neutrality and future social energy needs. Biomass liquefaction technology can convert low-grade renewable solid resources into high-grade liquid fuels and chemicals, and is the main method for efficient utilization of biomass. The commonly used methods for direct biomass liquefaction include hydrothermal liquefaction, atmospheric pressure catalytic liquefaction and ultrasonic/microwave assisted liquefaction. Although these liquefaction methods have been widely researched, they are normally suffered from the severe reaction conditions, significant energy consumption and/or high operational costs. Plasma is considered to be a new type of molecular activation technology due to its high chemical activity, which can induce the thermodynamic unfavorable chemical reactions at ambient condition. The effectiveness of using plasma for biomass liquefaction has been demonstrated in the previous studies. Plasma-enabled fast liquefaction has been proved to have satisfactory liquefaction yields with high energy efficiencies and high liquefaction rate compared with the other liquefaction technologies, due to the high reactivity of plasma reaction. Lignocellulosic biomass is one biomass resource with high abundance and low price, which has attracted remarkable attention in the plasma liquefaction of biomass. In this talk, recent work related to the plasma-enabled fast liquefaction of lignocellulosic biomass will be reported [1-3]. The influence of different processing parameters and the possible reaction mechanisms will be discussed. The future research directions will be proposed.

References

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[2] F. Liu, M.L. Cai, S.Y. Liu, et al. IEEE Access, 2020, 8, 2621-2630.
[3] S. Wang, S.Y. Liu, D.H. Mei, et al. Frontiers of Chemical Science and Engineering, 2020, 14, 763-771.

Structure and surface insight into a temperature-sensitive CaO-based CO_2 sorbent

Yongqing Xu, Bowen Lu, Cong Luo* and Liqi Zhang

State Key Laboratory of Coal Combustion, Huazhong University of Science and Technology, Wuhan 430074, P. R. China
*e-mail: cluo@hust.edu.cn

Calcium looping process is a prospective strategy to remove CO_2 from flue gas. However, the CO_2 capture capacity of the CaO-based sorbents would be spoiled severe over the repeated cycles. In this work, a kind of NaCl-modified CaO-based sorbents were prepared by a simultaneous hydration and impregnation process and explored for cyclic CO_2 capture by a simultaneous thermal analyzer. The promotion mechanism was discussed by electron microscope, X-ray diffraction, N_2 physisorption, X-ray photoelectron spectroscopy, and so on. Results showed that NaCl tailored the temperature sensitivity of CaO-based sorbents, and it was a good promoter to enhance the carbonation activity of CaO-based sorbents, especially under higher temperature modes. At higher temperatures, NaCl would cover the surface of CaO, and promote the CO_2 transportability in the modified sorbent, and then greatly improve the carbonation ability of the sorbents over the cycles. After 50 repeated cycles, the CO_2 capture capacity of "10 NaCl/CaO" still retained at 0.288 g/g and 0.237 g/g when carbonated at 650 °C and 750 °C, which were 2.05 and 2.63 times that of "$CaCO_3$ AR" respectively. Hence, the temperature-sensitive CaO-based sorbent promoted by NaCl shows a promising prospect for CO_2 capture from flue gas.

Keywords: Calcium looping, CO_2 capture, alkali salt promoting, carbonation kinetics, temperature-sensitive CO_2 sorbent

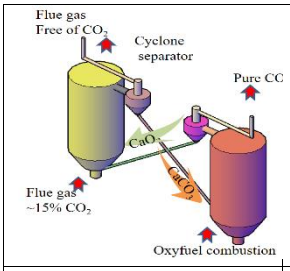


Figure 1. Calcium looping process for CO_2 capture

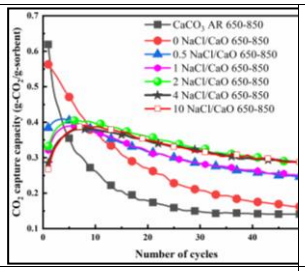


Figure 2. Cyclic CO_2 capture behavior of the NaCl modified sorbents with various Na: Ca ratios

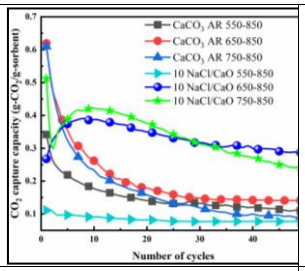


Figure 3. Cyclic CO_2 capture behavior of the NaCl modified sorbents at various carbonation temperatures (550-750 °C)

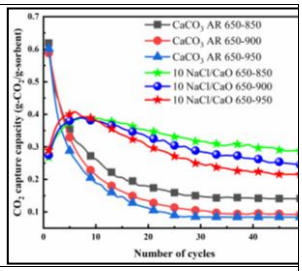
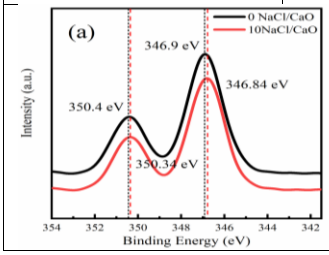
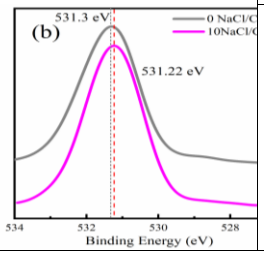
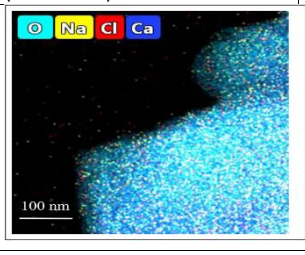


Figure 4. Cyclic CO_2 capture capacity of the NaCl modified sorbents at various calcination temperatures (850-950 °C)







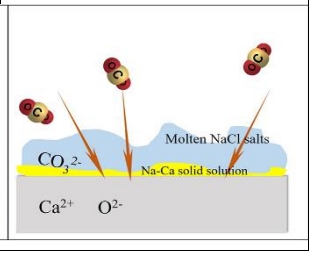


Figure 5. XPS spectra of the fresh "10 NaCl/CaO"(calcined at 600 °C for 5 hours): (a) Ca 2p3/2 and Ca 2p1/2; (b) O 1s	Figure 6. Schematic illustration of the enhancing mechanism of NaCl doped CaO-based materials

INTEGRATED ONE-STEP CO_2 ADSORPTION-CONVERSION PROCESS BY NON-THERMAL PLASMA

S. Xu[1,2,3*], X. Fan[2], H. Chen[2], C. Hardacre [2], R. A. Catlow[1,3,4]

[1] School of Chemistry, Cardiff University, Main Building, Park Place, Cardiff, CF10 3AT, UK
[2] Department of Chemistry, University of Manchester, Manchester M13 9PL, United Kingdom.
[3] UK Catalysis Hub, Rutherford Appleton Laboratory, Harwell, OX11 0FA, United Kingdom.
[4] Department of Chemistry, University College London, 20 Gordon Street, London, WC1H 0AJ, UK
*e-mail:shaojun.xu@manchester.ac.uk

Porous material, such as zeolites and metal-organic framework (MOF) materials show promise for the highly selective adsorption and separation of CO_2 at room temperature under both dry and humid conditions. However, the application of porous material-based catalysts in Integrated CO_2 capture and utilization (ICCU) process has been rarely explored, primarily due to the limited stability of MOFs against highly intense elevated reaction temperatures. Non-thermal plasma (NTP) activation can promote CO_2 conversion processes at room temperature by generating highly reactive species. Recently, NTP activation in porous material-based catalysts has been shown to enhance performance with the structure and porosity of the porous material being preserved. However, the efficient catalytic conversion of CO_2 into value added chemicals over porous material-based catalysts remains to be a highly challenging and important pipeline of research.

Here we report some recently developed examples of CO_2 capture over porous material-based catalysts at room temperature along with simultaneously NTP-activated direct conversion of CO_2. Porous material, such as zeolites and metal-organic framework (MOF) materials can significantly enrich the CO_2 concentration over the surface of the catalysts, then vastly facilitate the gas-phase and catalyst-surface reaction to convert CO_2 into value added chemicals. The integrated CO_2 utilization reactions are not limited to CO_2 direct decomposition into CO, but also CO_2 hydrogenation/reforming with molecular H_2/H_2O/CH_4 into a range of chemicals, including CO, CH_4, hydrocarbons and oxygenates (methanol, dimethyl ether, ethanol, etc). Compared with conventional thermal-based ICCU processes, NTP activation can effectively capture and one-through conversion of CO_2 into value added chemicals at room temperature.

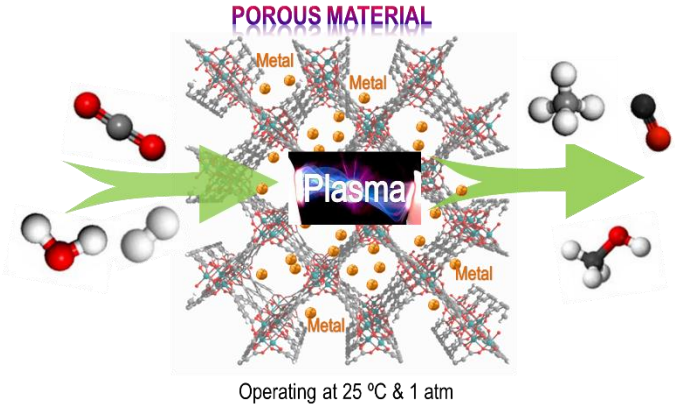


Figure 1. NTP-activated porous material-based catalysts for Integrated CO_2 capture and utilization.

IN SITU MOLECULAR IMAGING OF GREEN SOLVENTS FOR CO_2 CAPTURE

X.-Y. Yu[1,*]

[1] Oak Ridge National Laboratory, 5200, 1 Bethel Valley Rd., Oak Ridge, TN 37830, USA
*e-mail:yuxiaoying@ornl.gov

Switchable ionic liquids are emerging green solvents for carbon dioxide (CO_2) capture, cleaner separation, and efficient biomass production. However, the liquid structure and composition of SWILs are not fully understood. Besides off-line analyses using NMR and IR, our knowledge of the sustainable green solvents is limited. We used in situ liquid time-of-flight secondary ion mass spectrometry (ToF-SIMS) to study such solvents in this work. This is a unique molecular imaging technique enabled by the invention of a vacuum compatible microfluidic reactor SALVI. Green solvents were synthesized and reported previously. They were introduced into a vacuum compatible microfluidic channel for in situ analysis using liquid ToF-SIMS. Two model systems have been investigated. The first consists of 1, 8-diazabicycloundec-7-ene (DBU) and 1-hexanol with different CO_2 loadings. The second is primarily made of koechanol with various CO_2 loadings. Koechanol acts as both acid and base in the latter. Our results show two coexisting liquid phases in these green solvents. This phenomenon was only hypothesized in previous theory prediction. We were able to provide the first physical evidence of the complex liquid – liquid (l – l) interface using three-dimensional chemical mapping with submicrometer resolution. In addition, more complex stoichiometry is discovered due to CO_2 uptake. More importantly, we have provided the first chemical spatial visualization elucidating the evolving l – l interface. The more detailed molecular level understanding of the liquid structure and composition is instrumental to build the foundation for predicative material synthesis, CO_2 capture, and versatile applications.

CaO-based Materials for Integrated CO_2 Capture and Utilization

Hongman Sun[1, 2,*] and Chunfei Wu[2,*]

[1] College of Chemistry and Chemical Engineering, State Key Laboratory of Heavy Oil Processing, China University of Petroleum (East China), Qingdao, 266580, China

[2] School of Chemistry and Chemical Engineering, Queen's University Belfast, Belfast, BT7 1NN, UK

*e-mail:hongman.sun@upc.edu.cn; C.Wu@qub.ac.uk

Integrated carbon capture and utilization (ICCU) presents an ideal solution to address anthropogenic carbon dioxide (CO_2) emissions from industry and energy sectors, facilitating CO_2 capture and subsequent utilization through conversion into high-value chemicals, as opposed to current release into the atmosphere. Herein, we report the synergistic coupling of porous CaO, as a sorbent for CO_2 capture, and Ni doped CeO_2 nanorods, as catalytic sites for CO_2 reduction. It is found that ceria is shown to possess the capacity for CO_2 utilization, however, critically it only results in the generation of CO due to the weak CO-ceria bonding (Fig. 1). The addition of Ni active sites gives rise to CH_4 being the predominant product, via the strong interaction between Ni species and CO, which facilitates further reduction. Through tuning Ni loading, we have evaluated the role of catalytic active site size, with a Ni loading of only 0.5wt.% providing optimal performance through the formation of sub-nanometer sized clusters. This near-atomic active site dispersion gives rise to CH_4 productivity and selectivity of 1540 mmol g^{-1} Ni and 85.8%, respectively, with this optimal combination of catalyst and sorbent demonstrating high stability over 10 cycles of ICCU process. These observations in parallel with the synergistic coupling of earth-abundant, low-cost materials (CaO and Ni) will have broad implications on the design and implementation of high efficiency, cost-effective ICCU materials and processes.

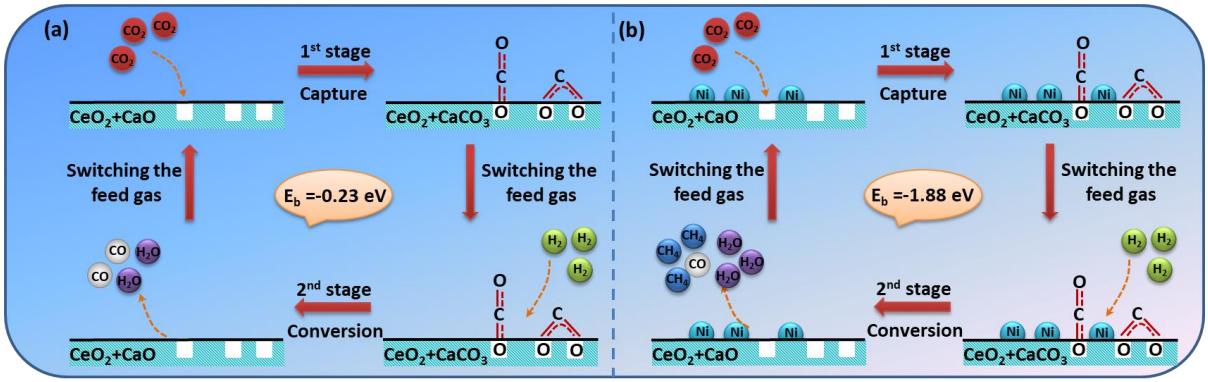


Fig. 1. Reaction mechanism during the ICCU process: (a) CeO_2-CaO, (b) Ni/CeO_2-CaO.

Closing both carbon and plastic loops towards a circular economy

X. Yuan[1,2*]

[1] Korea Biochar Research Center, APRU Sustainable Waste Management Program & Division of Environmental Science and Ecological Engineering, Korea University, Seoul, 02841, Republic of Korea
[2] R&D Centre, Sun Brand Industrial Inc, Jeollanam-do, 57248, Republic of Korea
*e-mail:yuan0125@korea.ac.kr

In addition to climate change, plastic pollution is widely recognized as one of the most severe environmental concerns. Waste plastic-derived advanced materials for carbon capture provide promising solutions to these environmental issues. However, the environmental sustainability and economic feasibility of such a novel approach are still unclear for it to be implemented on an industrial scale globally. In this talk, we investigated three synthesis routes to upcycle waste PET plastic into novel porous carbons for capturing CO_2 from both techno-economic and life-cycle perspectives. The one of major findings is that owing to the environmental benefits and economic feasibility of this approach, we highlighted its potential as a multifunctional alternative to conventional CO_2 absorption and plastic waste management technologies.

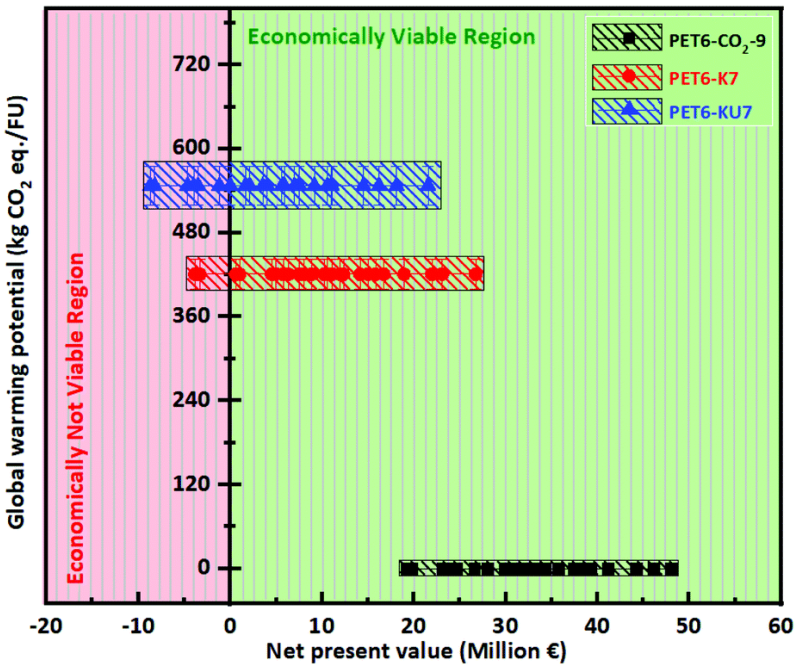


Fig 1. Environmental impact and economic benefit of the three waste plastic-derived porous carbons

Challenges for supported molten-carbonate membranes

G.A. Mutch[1,2*]

[1] Materials, Concepts and Reaction Engineering (MatCoRE) Research Group, School of Engineering, Newcastle University, Newcastle-upon-Tyne, UK
[2] Centre for Energy, Newcastle University, Newcastle-upon-Tyne, UK
*e-mail: greg.mutch@newcastle.ac.uk

Supported molten-salt membranes are emerging as promising CO_2 separation devices.[1] They recently overcame key performance targets required for economically competitive post-combustion CO_2 capture (CO_2 permeance (10^{-7} mol m^{-2} s^{-1} Pa^{-1}), CO_2 permeability (10^{-11} mol m^{-1} s^{-1} Pa^{-1}), CO_2/N_2 selectivity (>100)).[2] This performance is significantly beyond the dominant polymeric membrane class, and occurs at temperatures where polymer membranes are unstable, which may open exciting avenues in reaction engineering scenarios. However, due to their relatively earlier stage of development, challenges for supported molten-salt membranes include microstructural control and stability of support materials, characterization from the materials to device scale, and understanding permeation mechanism.

In this presentation, microfabrication strategies to produce high performance membranes, *e.g.* laser-drilling, directional solidification, phase-inversion, freeze-casting *etc*,[2-5] will be discussed in the context of the underlying theory on pore structure.[6] The utility of cutting-edge characterization, including 'whole device' X-ray micro-computed tomography, will be shown to provide unique insights into the temporal evolution of membrane structure.[2] Whereas the mobility of molten salts within the membrane structure raises questions about membrane sealing, manifolding, and molten salt creep, it will also be shown to be advantageous for producing autonomously and intrinsically self-healing membranes.[7] Moreover, strategies to control molten salt distribution within supports, and their impact on performance, will be discussed.[5] The advantages of using such microfabrication approaches in tandem with improved permeation measurements (*i.e.* well-defined driving forces *via* the use of permeant-containing sweep gases) will be presented as a call for the field to significantly improve the robustness and utility of permeation data.[4,5] Finally, recent results from near-ambient pressure X-ray photoelectron spectroscopy studies, and density functional theory calculations, will provide initial insights into molten salt speciation (and potentially permeation mechanism).

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CURRENT TRENDS AND FUTURE DIRECTIONS IN MEMBRANE BASED CO_2 CAPTURE

A.L. Khan[1*]

[1] Department of Chemical Engineering, COMSATS University Islamabad, Lahore, Pakistan
*e-mail:alaeeqkhan@cuilahore.edu.pk

Global emissions of carbon dioxide (CO_2) from industrial, agricultural, and domestic sources have been elevating over the years. At the end of 2020 global CO_2 concentration in the atmosphere was 412.5 ppm which is very drastic since the world has seen COVID-19 imposed lockdown and international decarbonization efforts (Paris agreement, COP26 etc.) CO_2 capture and storage (CCS) has long been considered a viable method of removing CO_2 from the atmosphere on a large scale. While conventional separation technologies including as absorption, adsorption, and cryogenic distillation have been utilized to capture industrially produced CO_2 for decades, their high energy requirements necessitate dire innovation for future CCS. Membrane-based techniques strives towards resolving high energy penalties by providing both technical and an economically viable substitute for CCS, by offering high energy efficiency, modularity, low maintenance, and continuous operation mode. Currently massive efforts are being focused to develop novel membrane materials including polymers ranging from conventional non-porous to advance porous materials, inorganics, supported liquids and novel two-dimensional laminar materials. Due to their inherent advantages, polymers are regarded as the most promising materials for the fabrication of gas separation membranes. However, polymeric membranes continue to confront significant limitations due to the trade-off between permeability and selectivity.

To circumvent trade-off constraints, several studies have been conducted in the past decades through different approaches. The concept of producing mixed matrix-matrix membranes by adding organic/inorganic fillers into the continuous polymer matrix has been extensively. Supported ionic liquid membranes comprising of a task-specific ionic liquid immersed in a porous substrate has shown promising results. In recent years, naturally occurring deep eutectic solvents have been employed in membranes as a greener and sustainable alternative to ionic liquids. Polymer modification and development of highly permeable and inherently selective polymers is another approach that has helped pushed the current limits. This study will provide a comprehensive overview of the most successful techniques, and provide brief highlights of the studies conducted by the Membrane Systems Research Group at COMSATS University.

Techno-economic Feasibility Analysis of Carbon Membranes for Integrated Biohydrogen Purification and CO_2 Capture

X. He[1,2,*], L. Lei[3], Z. Dai[4]

[1] Department of Chemical Engineering, Guangdong Technion Israel Institute of Technology (GTIIT), 241 Daxue Road, Shantou 515063, China

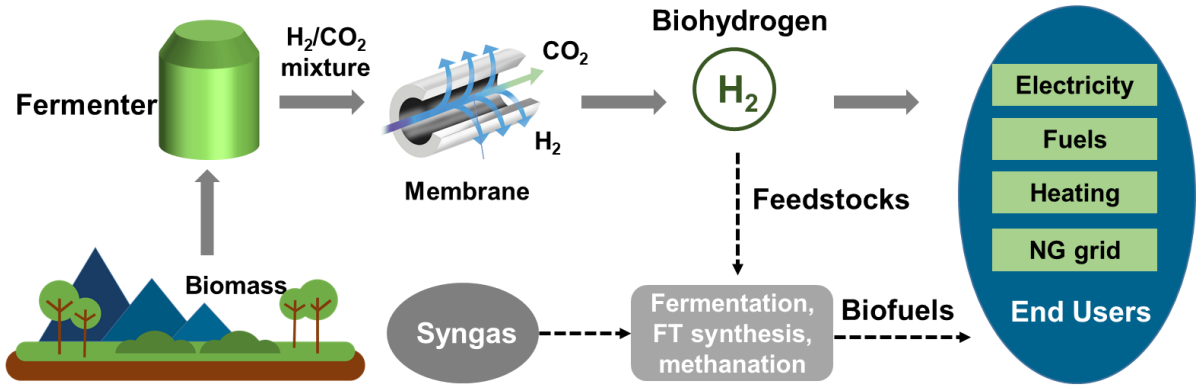
[2] The Wolfson Department of Chemical Engineering, Technion - Israel Institute of Technology, Haifa 3200003, Israel

3 State Key Laboratory of Chemical Engineering, School of Chemical Engineering, East China University of Science and Technology, 130 Meilong Road, Shanghai, 200237, China

[4] College of Architecture and Environment, National Engineering Research Centre for Flue Gas Desulfurization, Sichuan University, 24 south Section 1 Ring Road No.1 Chengdu 610065, China

*e-mail:xuezhong.he@gtiit.edu.cn

Abstract: Biohydrogen production from biomass by a fermentation process provides a great potential to achieve a green hydrogen economy for sustainable energy development. However, the purification of fermentative biohydrogen usually contains 30-40 vol.% CO_2 at small-scale plants requires advanced separation technologies. Carbon molecular sieving membranes are considered as an alternative solution in this application. This work focuses on the techno-economic feasibility analysis of H_2-selective carbon membrane systems for biohydrogen enrichment and CO_2 capture by investigation of process design, optimization of operating parameters, and the selection of membrane materials. High vacuum operation on the permeate is favorable to reduce the specific cost as the membrane-related capital cost is dominating the total cost. While feed gas compression provides better separation performance, and the minimum specific cost of \$0.026/Nm^3 at 6 bar was identified to achieve a hydrogen recovery of 90 %. A two-stage carbon membrane system was evaluated to be technically feasible to reach the biohydrogen purity of >99.5 vol% as fuels with the specific cost of \$0.06/Nm^3 purified biohydrogen, which is lower compared to PSA technology. The sensitivity analysis indicates that the membrane system is scalable and flexible in responding to the variation of plant capacity with the feed flow ranging from 500-2500 Nm^3/h without significant changes in production cost. Even though higher selectivity is required for membrane materials, the improvement of gas permeance by developing submicrometer asymmetric carbon membranes is urgently needed to enhance the competitiveness of this technology for integrated biohydrogen purification and CO_2 capture.


Fermenter
H_2/CO_2 mixture
CO_2
H_2
Membrane
Biohydrogen
H_2
Feedstocks
Electricity
Fuels
Heating
NG grid
End Users
Biomass
Syngas
Fermentation, FT synthesis, methanation
Biofuels

Amine-impregnated silica zeolite from microalgae ash at different calcination temperatures for CO_2 capture

Cui Quan

Xi,an Jiaotong University

Microalgae is an excellent type of biomass for bio-energy production due to its high calorific value and fast growth. However, a large amount of ash would be generated during microalgae utilization. In this work, MCM41 was prepared from microalgae ash. The materials were calcined at different temperatures (450oC, 500oC, 550oC, and 600oC), and the effect of calcination temperature was investigated. Polyethyleneimine (PEI) was loaded in MCM41 by the impregnation method at different loading amounts (30%, 40%, 50%, and 60%). The CO2 capturing capacity was measured. The results showed that the MCM41 calcined at 450 oC was the optimal material, which performed the most developed pore structure. Amine loading enhanced the CO2 capturing capacity of MCM41. The CO2 capturing capacity increased as PEI loading amount increased. The highest CO2 adsorption amount was 2.275 mmol/g with 60% amine loading at 25oC and 1 bar. Adsorption temperature had a mild impact on CO2 capture, and its CO2 adsorption amount decreased slightly with an increase in the adsorption temperature. It was considered that the CO2 uptake of amine-impregnated MCM41 kept stable at different temperatures below 100oC. Also, it showed good cyclic stability. After 10 cycles, the CO2 capturing capacity of 1.6 mmol/g was exhibited.

Submitted abstract

Application of carbon capture and storage technology in ultra-high performance concrete

HAN YI a, Xiao-Yong Wang a,b,*

a Department of Integrated Energy and Infra System, Kangwon National University, Chuncheon-Si, 24341, South Korea

b Department of Architectural Engineering, Kangwon National University, Chuncheon-Si, 24341, South Korea

*e-mail:hanyii@kangwon.ac.kr

At present, more and more countries worldwide have set carbon neutrality goals. In order to achieve this goal as soon as possible, the concrete industry also needs to promote new processes and technological innovations. In this study, gaseous CO_2 was converted into solid nano-calcium carbonate by CO_2 capture and storage technology and added to ultra-high performance concrete. The effect of NCC on the early performance of UHPC was investigated. The experimental results show that NCC can greatly accelerate the hydration reaction rate of UHPC. After adding 3% NCC, the compressive strength of UHPC at 1 day and 3 days was increased by 72% and 20%, respectively. Microscopic characterization analysis also confirmed that solid hydration products were formed more quickly after the addition of NCC.

Key words: CO_2 capture and storage, nano-calcium carbonate; heat of hydration, microscopic characterization

Effect of Boron Anomaly and Multi-electron Reactions on Lithiation Process of Amorphous Cathodes

Fanhou Kong

Queen's University Belfast and Hainan university

email:kongfanhou@163.com

As an emerging category of lithium ion battery cathode material, vanadium-based amorphous materials are far less understood in terms of the their performance and working mechanism as compared to the mature crystalline based lithium battery electrode material technologies. Compared with the mature state of the art of crystalline cathode materials for lithium ion batteries, amorphous cathodes face numerous and different challenges. This study explores the impact of the oxidation-reduction reaction process and Mo-V diatomic coupling on lithiation by introducing Mo2B as a reducing agent into the structure of V2O5-Li3PO4 glass. The results show that the mixed system simultaneously generated B2O3, MoO3 and VO2. With the increase of B2O3, the [BO3] triangle transforms into the [BO4] tetrahedron, accompanying by the boron anomaly effect, and V5+ transforms into V4+. 65V2O5-30Li3PO4-5BMo2 (VPBMo2) shows an excellent specific capacity, rate performance, structural stability and had the highest electronic conductivity. The lithiation mechanism of Mo6+/Mo4+conversion reaction is identified, and the V-Mo coupling multi-electron reaction is found to increase the specific capacity of the lithium ion battery. According to DFT calculations, the VPBMo2 has magnetism and becomes metallic. After Li adsorption, the peak density of states at the Fermi level increases, indicating that the conductivity of the VPBMo2 is enhanced. This strategy provides a new path for selecting suitable cathode materials for next-generation lithium ion batteries.

Enhancement of the production of hydrocarbon-rich fuel and high-quality bio-oil from corn stalk by Na2S2O8 pretreatment combined with rapid pyrolysis

Jiapeng Wang

Southeast University

Email:469527572@qq.com

As a carbon-neutral material, biomass has been widely studied and utilized in recent years. It is a green way to produce biomass fuel by pyrolysis. However, biomass is naturally resistant due to the high complexity in the component organization and interaction in the cell wall, which hinders the progress of pyrolysis. And the high oxygen content, strong acidity and low hydrocarbon content of pyrolysis bio-oil also weaken its application in renewable energy. In order to solve these problems, this study aims to propose a method for upgrading biomass pyrolysis products based on the combination of sodium persulfate pretreatment and rapid pyrolysis. Corn stalk was pretreated with sodium persulfate which activated by the coordination of UV lamp and heating to remove rigid components such as lignin in biomass, and then rapidly pyrolyzed to produce hydrocarbon-rich bio-oil. The result showed that after sodium persulfate pretreatment, the components of lignin were significantly reduced, the carbon dioxide, acid and oxygen-containing functional groups of the pyrolysis products were significantly reduced, and the phenolic content was increased. The yield of aromatic hydrocarbons and total hydrocarbons have a high value under the catalytic pyrolysis in the in the best performance. and the amount of yield reached 28.67% and 33.72%, respectively. Based on XRD, SEM, and FTIR analysis, it was also found that the biomass structure was destroyed and the components were gradually depolymerized which can let the biomass components move towards the reaction direction of lignin decomposition and cellulose/hemicellulose enrichment after sodium persulfate pretreatment. ICP result reflected that after sodium persulfate pretreatment, alkali metals and alkaline earth metals also had obvious removal effects. These results indicated that sodium persulfate pretreatment provides a new and effective method for biomass pyrolysis to produce high value-added chemicals and hydrocarbon-rich bio-oil.

Polymers of intrinsic microporosity for CO_2 separation and capture

Jiangtao Liu, Academic

University of Science and Technology of China

Email:jiangtaoliu@ustc.edu.cn

Traditional CO_2 capture processes such as pressure swing adsorption and cryogenic distillation are energy intensive. An alternative strategy to these conventional processes is membrane technology, which possesses typical advantages of low energy consumption, easy operation and maintenance, small footprint, and environmental friendliness. However, the main obstacles of the existing polymeric membranes on the way to full application on industrial scale are (1) achieving high gas permeability without sacrificing good gas selectivity, since permeability and selectivity usually exhibit a trade-off constraint, and (2) maintaining the long-term stability in gas separation performance by overcoming the problem of physical aging. PIM membranes show improved physical aging resistance in long term stability over 120 days compared with the pristine membranes, that's probably because the β-CD units can grasp the polymer chains via ether bonds, hold the architecture and make the highly rigid polymer networks unable to collapse. Since β-CD is one kind of commercially available organic materials, PIM-CD membrane is an attractive candidate for CO_2 separation and capture from flue gas and easy to scale up for industry application.

Transition metal cation-exchanged SSZ-13 zeolites for CO_2 capture and separation from N_2

Mingzhe Sun, Academic

The Hong Kong Polytechnic University (PolyU)

Email: mingzsun-c@my.cityu.edu.hk

CO_2 capture from post-combustion flue gas mixture (CO_2/N_2:15/85) is challenging and requires adsorbents with high capacity and high selectivity toward CO_2. Our work validated the potential of transition metal cation-exchanged SSZ-13 zeolites for efficient CO_2 capture, as evaluated by unary static isothermal adsorption and binary dynamic column breakthrough experiments as well as predicted performance in pressure/vacuum swing adsorption (P/VSA) process. Among the investigated transition metals (Co(II), Ni(II), Zn(II), Fe(III), Cu(II), Ag(I), La(III), and Ce(III)) exchanged SSZ-13, Co(II)/SSZ-13 and Ni(II)/SSZ-13 showed the highest CO_2 uptake (4.49 and 4.45 mmol/g, respectively) and superior selectivity of CO_2 over N_2 (52.55 and 42.61, respectively) at 273 K and 1 atm. We attribute such outstanding separation performance to the Pi backdonation exclusively formed between CO_2 and transition metal cation sites. This demonstrates a new approach of developing adsorbents for CO_2 capture in the real-world industrial processes.

Current Trends and Future Directions in Membrane based CO_2 Capture

Asim Laeeq Khan

University Islamabad

Email: alaeeqkhan@cuilahore.edu.pk

Global emissions of carbon dioxide (CO_2) from industrial, agricultural, and domestic sources have been elevating over the years. At the end of 2020 global CO_2 concentration in the atmosphere was 412.5 ppm which is very drastic since the world has seen COVID-19 imposed lockdown and international decarbonization efforts (Paris agreement, COP26 etc.) CO_2 capture and storage (CCS) has long been considered a viable method of removing CO_2 from the atmosphere on a large scale. While conventional separation technologies including as absorption, adsorption, and cryogenic distillation have been utilized to capture industrially produced CO_2 for decades, their high energy requirements necessitate dire innovation for future CCS. Membrane-based techniques strives towards resolving high energy penalties by providing both technical and an economically viable substitute for CCS, by offering high energy efficiency, modularity, low maintenance, and continuous operation mode. Currently massive efforts are being focused to develop novel membrane materials including polymers ranging from conventional non-porous to advance porous materials, inorganics, supported liquids and novel two-dimensional laminar materials. Due to their inherent advantages, polymers are regarded as the most promising materials for the fabrication of gas separation membranes. However, polymeric membranes continue to confront significant limitations due to the trade-off between permeability and selectivity. To circumvent trade-off constraints, several studies have been conducted in the past decades through different approaches. The concept of producing mixed matrix-matrix membranes by adding organic/inorganic fillers into the continuous polymer matrix has been extensively. Supported ionic liquid membranes comprising of a task-specific ionic liquid immersed in a porous substrate has shown promising results. In recent years, naturally occurring deep eutectic solvents have been employed in membranes as a greener and sustainable alternative to ionic liquids. Polymer modification and development of highly permeable and inherently selective polymers is another approach that has helped pushed the current limits. This study will provide a comprehensive overview of the most successful techniques, and provide brief highlights of the studies conducted by the Membrane Systems Research Group at COMSATS University.

Effects of Environmental conditions and nano particles on perfomance of PV panels

Nithin K C

Nitte Meenakshi Institute of Technology

Email: kcnithin17@gmail.com

A work in renewable energy sources is significant due to depletion of fossil fuels, environmental degradation and global warming related to fossil fuel. The renewable energy sources are renewed by the nature and operating cost is low. The solar energy is most widely used renewable energy source and the popular solar photovoltaic and solar thermal systems are used for solar energy conversion. The solar photovoltaic (PV) system converts the solar energy into electrical energy directly. The performance of the solar photovoltaic system is affected by ambient temperature, humidity, sola.

Plasma-catalytic dry reforming of methane over Ni/boron nitride catalysts

Yuanling Li

College of Environmental Science and Engineering, Nankai University

Email: m15620705341@163.com

Non-thermal plasma (NTP) coupled with catalysts provides a potential alternative to enable the dry reforming of methane (DRM) reaction at low temperatures. However, the catalytic efficiency of plasma-catalysis system remains lower than that of thermal catalysis system. Therefore, developing effective strategies to optimize the catalytic performance of non-noble metal-based catalysts in terms of activity and stability is a critical challenge for plasma-enabled DRM reaction. In this study, DRM over Ni/BN catalysts with different synthesis methods (BN_IPA_Ni, BN_DMF_Ni: preferential sonication of h-boron nitride (h-BN) by dispersants isopropanol (IPA) or N,N-Dimethylformamide (DMF), followed by loading of Ni ions; BN_Ni_IPA, BN_Ni_DMF: preferential loading of Ni ions on h-BN, followed by sonication with dispersants IPA or DMF) were investigated in a dielectric barrier discharge (DBD) plasma-catalysis system. Among, BN_IPA_Ni exhibited superior catalytic performance in terms of 40.5 % CH4 conversion, 26.6% CO_2 conversion, 9.3 % H_2 yield and 10.5 % CO yield. Its superior catalysis activity and stability should be attributed to the development of B-O defects, which was found to play a significant role in regarding the size control of Ni particles to facilitate the dissociation of H^* from CH4. In addition, the abundant B-O defects of BN_IPA_Ni assisted in eliminating excess CHx species for inhibiting the nucleation growth of carbon species to inert carbon.

Molecular simulation of CO_2 capture in amine-modified zeolite 13X

Ming Zhang

China University of Petroleum(East China)

Email:ZMklgz@163.com

There is a great need to synthesize high-performance adsorbents for potential application in post-combustion CO_2 capture. In this study, the CO_2 adsorption of zeolite 13X loaded with different amine (diethylenetriamine (DETA), triethylenetetramine (TETA), pentaethylenehexamine (PEHA)) from flue gas was studied by molecular simulation. The separation performance of amine-modified zeolite 13X was evaluated in detail in terms of adsorption isotherms, adsorption heat, adsorption sites and CO_2/N_2 selectivity. The simulated results showed that CO_2 molecules were preferentially adsorbed near the loaded amine, and the adsorption capacity and heat of CO_2 pure gas are significantly higher than that of 13X. 13X-DETA-9 exhibited a higher CO_2 loading and higher CO_2/N_2 selectivity, was the most promising adsorbent. At 348K and 0.3MPa, the CO_2 loading capacity of 13X-DETA-9 was 42.3% higher than that of 13X, and the CO_2/N_2 selectivity of 13X-DETA-9 was 1.94 times higher than 13X. Through molecular simulation study, the details and mechanism of CO_2 adsorption and separation in amine-modified zeolite 13X can be understood in micro-level, which provides guidance for experimental design and synthesis of high-performance CO_2 adsorbent.

Solvothermal liquefaction of waste Kariba weed into value-added products

Elfina Azwar

Universiti Malaysia Terengganu

Email: elfina.azwar@gmail.com

Aquatic weeds pose hazards to aquatic ecosystems and particularly the aquatic environment in shellfish aquaculture due to its excessive growth covering entire freshwater bodies, leading to environmental pollution particularly eutrophication intensification, water quality depletion and aquatic organism fatality. In this research, Kariba weed was transformed into value-added products for potential use as biofuels using solvothermal liquefaction approach. Solvothermal liquefaction is a thermochemical process that converts wastes into value-added products under high pressure. The char product was discovered to have high HHV value (29 MJ/kg) and carbon content (73 %). This indicates that solvothermal liquefaction has the potential to convert waste Kariba weed into an alternative fuel source.

Development of Li4SiO4 pellets using extrusion–spheronization technique for cyclic CO_2 capture

Hailong Li, Academic

School of Energy Science and Engineering, Central South University

Email: hailong_li@126.com

Carbon capture and storage (CCS) which can reduce the emission of carbon dioxide (CO_2) by sorbents is an excellent strategy for carbon neutrality. Lithium orthosilicate (Li4SiO4) is considered as a splendid sorbent for CO_2 capture due to its high adsorption capacity, low regeneration temperature and outstanding cyclic durability. However, the abrasion of Li4SiO4 sorbent in circulation fluidized-bad would result in a decrease in adsorption performance. To solve the problem, extrusion–spheronization technique was applied to convert the state of Li4SiO4 from powdery to spherical for better mechanical properties. On the hand, the extrusion probably reduce the porosity of the sorbent, thus pore-forming material should be introducing to overcome this advantage. In this work, we developed a low-cost and high porosity rise husk templated Li4SiO4 pellets, which effectively utilizes solid waste resources. The quick release of combustion gases from burning rice husk could increase surface area and porosity of the pellets. The 20 wt% rice husk-templated Li4SiO4 exhibited the capacity of 0.21 g/g, which was nearly twice than that of unmodified pellets. Furthermore, the alkaline compositions in rice husk promoted the formation of molten phases, which decreased CO_2 diffusion resistance. To test the feasibility for industrial applications, the mechanical properties of the Li4SiO4 pellets were also characterized. The maximum force that pellets could be sustained is 3.8 N which exceeded the minimum value (1 N) for large-scale industrial processes. This work may provide a methodology for simultaneously utilizing solid waste and modifying the mechanical and adsorptive properties of Li4SiO4 as an efficient sorbent in CO_2 capture technology.

Construction of Asymmetric Mixed Matrix Membranes Based on Ionic Liquids and Characteristics of CO_2 Separation

Shaohan Lian

Tianjin University

Email: shaohan_lian@163.com

In recent years, global warming caused by the greenhouse effect and a series of secondary events have attracted widespread attention, such as the California fire in the United States in 2020 and the floods in Henan, China in 2021, etc. CO_2 capture, utilization and storage technology (CCUS) has been widely recognized as an important way for human to deal with climate change and achieve carbon neutrality. Membrane separation technology is considered to be the most promising CO_2 capture technology due to its high efficiency and economy. Therefore, it is of great significance to develop high-efficiency CO_2 separation membrane materials. A novel mixed-matrix membrane with an asymmetric structure was developed based on solvent-directed induction. Under the synergistic effect of multiple factors, including additional facilitated delivery channels provided by amino acid-based deep eutectic solvent (ADES) and asymmetric membrane structure, the mixed matrix membrane exhibits excellent gas separation performance. Compared to pristine Pebax membranes, the CO_2 permeability is almost unaffected (only 0.6% lower) while the CO_2/N_2 selectivity is increased by 17%. The improvement effect of this method in other polymer-based membranes is also obvious, indicating that this strategy has the potential to break through the "trade-off" effect. In addition, the interaction mechanism between the composite membrane and gas molecules was studied by density functional theory (DFT) calculations, and the mechanism of gas transport across the membrane was analyzed from the microscopic scale.

Integration of Membrane Separation with Non-Thermal Plasma (NTP) Catalysis: A Proof-of-Concept for CO_2 Capture and Utilisation (CCU)

Huanhao Chen, Academic

State Key Laboratory of Materials-Oriented Chemical Engineering, College of Chemistry and Chemical Engineering, Nanjing Tech University

Email: h.chen@njtech.edu.cn

Carbon dioxide (CO_2) capture and utilisation (CCU) plays an important role in abating carbon emissions, mitigating global warming and converting CO_2 as feedstock to value-added fuels and chemicals. Herein, a proof-of-concept study of a novel integrated process, consisting of a membrane separator (MS) followed by a non-thermal plasma reactor (NTPR) in tandem, was presented and systematically investigated, as an efficient platform, for potential applications in CCU. Specifically, biogas upgrading via CH4 enrichment was used as the model system to investigate the proposed integrated system (using SAPO-34 zeolite membrane in MS and Ni/NaBETA and Ni/UiO-66 catalyst in NTPR). Upon optimisation, the hybrid MS-NTPR system showed satisfactory carbon capture efficiency (CCE) and carbon utilisation efficiency (CUE) of ca. 91.8% and 71.7%, respectively. In addition, the integrated process also exhibited excellent stability for CCU in upgrading synthetic biogas with a stable performance over a 40-h longevity test. This work, for the first time, showed the feasibility of using the novel integrated process for effective CCU.

Rational Design of Mixed Matrix Membranes with Metal-Organic Polyhedra for CO_2/N_2 separation

Fan Chen

Texas A&M University

Email: fancheN2018@tamu.edu

Mixed matrix membranes (MMMs), composed by polymer matrix and inorganic fillers, are competitive candidates for post-combustion CO_2 capture. As a combination, MMMs possess the fortes of both components, flexibility and workability of polymer matrix and porosity and selectivity of inorganic fillers, resulting enhanced permeability and selectivity. However, the poor interface compatibility between those two phases, like void defects etc. is a dominant challenge to achieve higher gas separation performance. Here we report a facile method to manufacture homogeneous MMMs for CO_2/N_2 separation by utilizing metal-organic polyhedra (MOPs) as the fillers. The dissolvable nature of MOP cages is the key to realize molecularly dispersion of fillers, thus eliminating the poor interface compatibility. To be detailed, we incoporated one kind of CO_2 selective MOP, UMC-1, with poly(ethylene glycol) diacrylate (PEGDA). Several technical processes were applied to obtain the uniform liquid mixture that underwent UV illumination for a crosslinking reaction of the PEGDA matrix, leading to flexible, even, thickness-adjustable MMMs. With MOP loading increase in an optimal range, MMMs showed improvement on both permeability and selectivity. For example, after the addition of only 1 wt% UMC-1 to PEGDA, the CO_2 permeability enhanced from 77 Barrer to 102 Barrer and CO_2/N_2 selectivity improved from 60 to 92. MMMs with 3 wt% UMC-1 were tested to have the best performance, exhibiting an ideal selectivity at 112.6 with CO_2 permeability at 64.0 Barrer. These MMMs exceeded the 2008 Robeson upper bound, which is a trade-off between permeability and selectivity for traditional pure polymer membranes, demonstrating a very promising platform for carbon capture and other challenging applications.

Superior selective CO_2 adsorption and separation over N_2 and CH4 with porous carbon nitride nanosheets

Zhao Li

China university of petroleum-Beijing

Email: 15232185100@163.com

Driven by accelerating energy demand, the global warming issues have become one of the main climate concerns around the world.1–3 Facing the challenge requires technological investigation to decrease the CO_2 which is the main by-product in the process of carbon-based fuels consuming.4,5 Moreover, as a valuable feed tock, CO_2 is also of prime importance in fine chemicals, pharmaceuticals, food packaging, agricultural production and polymers.6 Thus, it is necessary to develop gas cleaning technology for capturing the CO_2 from natural gas, biogas and landfill.7,8 Traditional technology applied in the mixture gases separation were cryogenic distillation and amine absorption, but both of them suffered from energy consumption, toxicity, and severe equipment corrosion.9,10 Considering energy cost of operation, physical adsorption has received much attention owing to its high efficiency and sustainable regeneration.11–13 It was worthy to choose and develop suitable adsorbent with high gas adsorption capacity and selectivity for further investigation. As the urgent demand for CO_2 capture, diverse adsorbent materials have been continuously explored, such as porous activated carbons,14–17 porous organic polymers,18,19 metal-organic-frameworks20–23 and carbon nitrogen materials24–26. However, this is challenging for high CO_2 adsorption and selectivity at ambient temperature and pressure. Notwithstanding many practical obstacles, recent advances have been achieved in the graphite slit which possesses controllable interlayer space and highly accessible surface area. More importantly, water as an inevitable composition (taken up 10% molar concentration) of real flue gas mixtures whose influence on the process of gas adsorption should be taken seriously. Owing to a competitive relationship between water and CO_2 molecules, the adsorbent became instability and even collapse because of the existence of water when the CO_2 interacted with the adsorbent.Development of high-performance materials for the capture and separation of CO_2 from the gas mixture is significant to alleviate carbon emission and mitigate the greenhouse effect. In this work, a new model of C9N7 slit was developed to explore its CO_2 adsorption capacity and selectivity using Grand Canonical Monte Carlo (GCMC) and first-principle density function theory (DFT) calculations. Among varying slit widths, C9N7 with the slit width of 0.7 nm exhibited remarkably CO_2 uptakes and also with superior CO_2/N_2 and CO_2/CH4 selectivity. At 1 bar and 298 K, a maximum CO_2 adsorption capacity can be obtained as high as 7.06 mmol/g and the selectivity of CO_2/N_2 and CO_2/CH4 was 41.43 and 18.67, respectively. In the presence of H_2O, the CO_2 uptake of C9N7 slit decreased slightly as the water content ratio increased, showing a better water stability. Furthermore, the underlying mechanism of highly selective CO_2 adsorption and separation on the C9N7 surface was revealed. The closer the adsorption distance, the stronger the interaction energy between the

gas molecule and C9N7 surface. Finally, in order to better understand the mechanism of highly selective CO_2 adsorption and separation on the C9N7 slit, we elaborated the CO_2 adsorption energy and behaviors in the presence of N_2, CH4, and H_2O by DFT calculations. Above all, the strong interaction between C9N7 nanosheets and CO_2 molecules contributes to its impressive CO_2 uptake and selectivity, suggesting that the C9N7 slit could be a promising candidate for CO_2 capture and separation.Keywords: C9N7 membrane; CO_2 adsorption and selectivity; water stability; density function theory; Grand Canonical Monte Carlo.

A review on role of Ruthenium (Ru) based catalyst in CO_2 Capture and hydrogenation reactions

Khushbu G. Patel, Academic

Rai University, Ahemedabad, Gujarat, INDIA

Email: patelkhushbug09@gmail.com

The effective strategies in dealing with current environmental issues are to development of sustainable energy technologies and reduction of carbon dioxide in the atmosphere. To mitigate environmental concern and energy issues, the conversion of carbon dioxide (CO_2) to valuable and useful chemicals offers a promising strategy for the development of a carbon neutral economy. This review aims the recent progress on CO_2 capture and in situ catalytic transformation. The contents are introduced according to the Ru based catalysts, in which different reaction type is involved and the transformation mechanism of the captured CO_2 and the role of Ru based catalyst in the conversion other value-added products are especially elucidated.

Charge-modulated adsorption and separation of CO_2 over N_2 on carbon nitride nanosheets: Insights from GCMC simulations

Zilong Liu, Academic

China University of Petroleum-Beijing

Email: zilong@cup.edu.cn

The efficient separation of CO_2 over N_2, particularly at ambient temperature and pressure, is a key factor in the capture of carbon from flue gas. In this work, for the first time we investigated the CO_2 adsorption on C9N7 nanosheet with different charge states by means of Grand canonical Monte Carlo (GCMC) simulations. It was found that the adsorption capacity of CO_2 was much stronger than that of N_2. At 298 K and 1 bar, the CO_2 adsorption capacity of the C9N7 is 8.42 mmol/g, whereas the N_2 absorption capacity is only 1.02 mmol/g. Increasing the applied negative charge, adsorption capacity of CO_2 greatly increased, reaching 28.62 mmol/g with a charge of 60 e. The selectivity analysis showed that the selectivity of the C9N7 with 60 e to CO_2/N_2 is up to 200 at 298 K. The higher the pressure, the higher the selectivity of CO_2 adsorption. Additionally, the temperature effect indicated that the C9N7 membrane can be recycled and served as an excellent candidate for CO_2/N_2 separation at ambient conditions. The obtained results provide useful guidance for developing advanced materials and applying new regulation techniques to realize highly tunable and selective CO_2 capture and separation.

Study on CO_2 Reduction Based on Metal-supported 3D SiO2 Coupled with Low Temperature Plasma

Jiahan Yang

North China Electric Power University

Email: 931052282@qq.com

This article introduces the hazards of CO_2, a gaseous pollutant, and outlines methods and technologies for reducing CO_2. The research status of the catalytic reduction of CO_2 with DBD coupled catalyst is reviewed. The application of the three-dimensional structure catalyst in various fields has been investigated in detail. The method of DFT calculation and screening for preparing new catalysts was investigated and researched. The results show that the use of DFT simulation calculation to prepare a new type of three-dimensional structure catalyst combined with low-temperature plasma reduction of CO_2 has good research value and application prospects.

Keywords: three-dimensional structure; low-temperature plasma; CO_2 reduction; simulation calculation screening

Multi-objective optimization and decision-making of Temperature Swing Adsorption cycle performance for CO_2 capture

Jiajun Wang

Tianjin University (Key Laboratory of Efficient Utilization of Low and Medium Grade Energy)

Email: m13842557704@163.com

The increase in CO_2 emissions is causing a number of environmental problems such as global warming and it is urgent to reduce CO_2 emissions. The widely studied adsorption method of carbon capture technology lacks the studies related to cycle performance optimization and decision making that take into account multiple objectives at this stage. Temperature swing adsorption (TSA) is used as the research object in this paper. The cycle performance optimization and decision-making algorithm are established combining the method of machine learning to conduct multi-objective optimization and decision-making research on cycle performance under different performance weight requirements. The results show that: the artificial neural network (ANN) model obtained by the machine learning method can accurately represent the cycle performance under different operating parameters. A competitive relationship is shown throughout between yield and exergy efficiency, a dual relationship of both competition and positive correlation exists between recovery and exergy efficiency. And a perfectly positive relationship is shown between purity and recovery. The results of the decision when balanced cycle performance is used as the demand guide show that the cycle performs poorly in terms of the efficiency of the cycle.

Insights into solvent effect guiding the fabrication of highly performance mixed-matrix membrane for CO_2 separation

Boyu Li

Tongji University

Email: liboyuxiaopang@126.com

Solvent effect plays a significant role in developing a proper chemical reaction process. In this paper, polyaniline (PANI)-modified MOF (Cu-BDC) was prepared with three common organic solvents (DMF, DMSO, and NMP) via post-synthesis method (PSM) to understand the role of solvation in synthesis the hybrid structure of polymer-MOF particles. The results show that DMF is more suitable for chemical reactions due to strong hydrogen bonding and good solubility. The PANI-modified Cu-BDC with DMF (Cu-BDC-F@PANI) was then successfully dispersed in poly (vinylidene fluoride) (PVDF) to fabricate mixed-matrix membranes (MMMs) Cu-BDC-F@PANI/PVDF, which displays regular shape and homogeneous channel structure. Cu-BDC-F@PANI/PVDF shows a good performance in CO_2/N_2 gas separation experiments, with permeability coefficient of 1130.7 Barrer, higher than the other two MMMs (Cu-BDC-O@PANI/PVDF, Cu-BDC-P@PANI/PVDF) based on DMSO and NMP solvents, respectively. Meanwhile, the permeability of Cu-BDC-F@PANI/PVDF is about 188.5, 208.2, 128.5 times higher than the commercial membranes (cellulose acetate, polysulfone, polycarbonate). The excellent ideal construction and strong interaction due to chemical activity between PANI and CO_2 explains the transmembrane mechanism of electrostatic interaction and acid-base neutralization. Moreover, the Cu-BDC-F@PANI/PVDF membrane with excellent reproducibility has long-term stability for CO_2 separation performance over 21 days.

High-Performance Single and Bimetallic Desulfurization Adsorbents with Abundant Active Sites Prepared from Phytoremediation

Li Weining

State Key Laboratory of Heavy Oil Processing, College of Chemical Engineering, China University of Petroleum (East China)

Email: li_weining426@163.com

Phytoremediation can degrade heavy metals in wastewater and disperse heavy metal ions uniformly throughout the plant. The adsorbent prepared by pyrolyzing the plant has the advantages of uniform metal loading and small metal particles. However, its applicability and practical significance have not been verified. Therefore, in this study, Pistia stratiotes were cultivated in Fe, Ni, Co, Cu, Zn, Ce, and Mg solutions with the same concentration; among them, Ni, Co, and Cu single-metal desulfurization adsorbents (ACA-I) had better adsorptive desulfurization performance. Furthermore, it was cultivated in three metal solutions, such as Ni-Co, Ni-Cu, and Co-Cu, to obtain bimetallic desulfurization adsorbents (ACA-II). The TEM and SEM mapping results showed that the dispersity of metal particles and the diameter of metal particles on the surface of the ACA-II were better. The adsorptive desulfurization performances of PSLAC-Co-Ni, PSLAC-Cu-Ni, and PSLAC-Co-Cu are 87 mg g-1, 83 mg g-1, and 80 mg g-1, respectively, which are better than those of ACA-I. This indicates that this study is not only applicable to simple single-metal solution systems but also more complex bimetallic solution systems. This study solves two major environmental problems of heavy metal pollution in water and excessive sulfur content in fuel oil, playing a dual role in promoting environmental protection.

Water effect on adsorption carbon capture in metal organic framework: a molecular simulation

Long Jiang, Academic

Zhejiang University

Email: jianglong@zju.edu.cn

Considering water vapor is a component in almost all CO_2-rich industrial gas streams, it is of critical importance to understanding interaction mechanisms between adsorbents and adsorbates. This paper aims to comprehensively analyze water effect on CO_2 adsorption for metal-organic framework (MOF) in a broad working pressure range which may bring some new insights based on a molecular simulation. First, Mg-MOF-74 is selected and synthesized according to previous literature. Equilibrium adsorption capacitys and enthalpies are obtained by grand canonical Monte Carlo (GCMC) simulations, and the results for high-pressure CO_2 adsorption are validated by magnetic suspension balance experiment. It is indicated that there are three adsorption stages for pure CO_2 and four adsorption stages for pure H_2O under different pressure. Adsorption enthalpy also varies with adsorption capacity, which is fully explained from the angle of adsorption stages and adsorption energies. Further simulations of flue gas (CO_2/H_2O/N_2) adsorption at different humidities are carried out, and selectivity between CO_2 and H_2O is analyzed. Adsorption density distributions, simulation snapshots, and radial distribution functions are used in analysis processes, providing a general perspective for analyzing CO_2 adsorbents in the presence of H_2O.

Engineering the Micro-structure for Energy Consumption in Post-combustion Carbon Capture and Utilization Process

Yanli Sun

North China Electric Power University

Email: sunyanli795@163.com

The dramatic increase in the concentration of CO_2 in the atmosphere of the earth has caused severe global extreme climate changes. In the past decades, CO_2 capture and utilization technologies have made great progress, which not only seals and stores CO_2 but also converts it into chemical fuels to mitigate the energy crisis and environmental issues. However, there are few works elaborating the relationship between surface/interface microstructure and macroscopic energy consumption at the molecular level in the field of science-engineers. Thus it is necessary to summarize this scope to point out the next-step research direction and focus. In this review, as for the simulation of industrial ultra-low emission flue gas in the flow phase and material regeneration, the surface/interface structure has a great effect on the regeneration consumption energy of CO_2 absorption/adsorption or the driving operation energy consumption in the catalytic process (including photocatalysis, electrocatalysis, thermal catalytic hydrogenation, photothermal catalysis, plasma catalysis). Based on this unique angle of view, the industrial/commercial feasibility of CO_2 capture and catalytic conversion technology was evaluated. Simultaneously, it is critical to declare the relationship between the surface/interface microstructure and energy consumption. With our great effort, this work would systematically introduce the CO_2 capture and catalytic conversion technology designed from the molecular level with low energy consumption, low cost, and efficient recycling. From our perspective, it is believed that balancing the structure design and energy consumption will benefit the practical application of CO_2 technology. This review would be of significance to give the direction to the academic researchers for obtaining an overall understanding of the relationship between micromaterials science and the macro-energy engineering scope.

The Origin of Superhigh CO_2 Reduction Activity with Transition Metal-based Photocatalysis: Reconstructed structure of the active site

Yuying Pang

Department of Environmental Science and Engineering, North China Electric Power University (Baoding)

Email: 572900403@qq.com

Solar-energy-driven carbon dioxide (CO_2) conversion to value-added chemicals emerged a highly desirable process to alleviate current environmental and energy problems. Recent decades have witnessed remarkable progress on upgrading of CO_2 reduction using photosensitized cobalt-based catalysts .Most studies focused on designing the material morphology and the number of active site in spatial distribution, regulating intrinsic coordination environment and optimizing of surface catalytic site geometry to improve th catalytic properties. These strategies mainly affected the electronic state density, coordination saturation and symmetry of coordination atoms. Additionally, environmental species adsorbing on the unsaturated coordination catalytic site, would change the symmetry of the original geometric structure of the the catalytic site, resulting in surface reconstruction.The new active site usually has better catalytic activity and selectivity.To date, the reconstruction of surface-active site during photocatalytic reaction and their roles in the chemical turnover remains ambiguously understood.In our study, DFT calculation showed that the CoOx active site generated by surface reconstruction of Co based catalyst could improve the adsorption performance of CO_2 and reduce the activation energy barrier of COOH*. Subsequently, Co based catalysts were prepared and photocatalytic tests were carried out.The test results agreed with the calculated results. CO_2-TPD, XPS, XAS and in situ Raman were used to observe the reconstruction of the catalysts and elucidate the improvement of catalytic performance.

Hydrothermal conversion of pectin under a temperature-pressure independent process

Shijie Yu

Tsinghua University

Email: yusj18@mails.tsinghua.edu.cn

Hydrothermal conversion can convert biomass into carbon materials in catalysis, energy storage, and water purification. Pectin, a polysaccharide widely presented in plant cell walls, is an important component of biomass. However, the formation and evolution of pectin-derived hydrothermal carbon are not clear. In this study, we conducted the hydrothermal treatment of pectin at 100–300 ?C to investigate the properties at different hydrothermal stages. With the characterization of the solid products with scanning electron microscopy (SEM), elemental analysis, N_2 adsorption/desorption, Fourier-transform infrared (FTIR) spectroscopy, Raman spectroscopy, X-ray photoelectron spectroscopy (XPS), and pyrolysis behavior in thermogravimetric analyzer (TGA), we proposed the formation and evolution pathway of pectin-derived hydrothermal carbon from original pectin. Pectin first underwent a physical change of gelation during the hydrothermal process, and then was hydrolyzed to liquid monomers. Pectin-derived hydrothermal carbon was formed by the polymerization of liquid monomers resulting from the hydrolysis of pectin. Moreover, the hydrothermal carbon was further carbonized, accompanied by dehydration and aromatization. Meanwhile, the originally irregular pectin bulk structure was completely transformed into carbon spheres above 200 °C. This work can provide some fundamental guidance for the sustainable synthesis of carbon materials from the hydrothermal process of pectin.

Bio-inspired CO_2 capture and simultaneous mineralization using polydopamine as crystal growth modifier in an aqueous system

Dharmjeet Madhav

KU Leuven, Belgium

Email: dharmjeet.madhav@kuleuven.be

Two major challenges in CO_2 mineralization in aqueous systems are (1) lack of efficient process, and (2) limited applications of produced carbonates. Here, we present a one-step convenient CO_2 capture and mineralization method to produce functional calcium carbonate (CaCO3) particles. We used a gas diffuser reaction setup to bubble CO_2 in liquid media containing reagents such as CO_2 absorption promotor, a bio-based water-soluble polymer polydopamine as crystal growth modifier, and Ca2+ ions. In the first step, the effect of CO_2 flow rates on Ca2+ conversion and particle morphology was investigated. Then, different concentrations of polydopamine with a fixed CO_2 bubbling rate were investigated for their effects on particle crystallization and growth. Finally, at optimized polydopamine concentration, the effect of different CO_2 bubbling rates was investigated. The functional carbonates that are produced by bio-inspired polymer mediated crystallization could be used as dye, heavy metals adsorbent, and functional composite fillers. Furthermore, the method could be used for CO_2/Ca2+ rich industrial waste valorization.

One-step fabrication of size-controllable, biowaste-templated Li4SiO4 spheres via freeze-drying method for cyclic CO_2 capture

Yuandong Yang, Academic

Shandong University

Email: yyd@sdu.edu.cn

High-temperature cyclic CO_2 capture based on Li4SiO4 adsorbent has drawn extensive attentions in recent decades. Especially, the fabrication of Li4SiO4 adsorbent pellets with sufficient mechanical strength has been considered as an essential precondition for achieving its practical looping application. In this work, size-controllable Li4SiO4 spheres were one-step fabricated via a novel freeze-drying method. And a typical industrial biowaste, bagasse, was employed as a low-cost and carbon-neutral pore-forming agent to enhance the CO_2 capture performance of freeze-dried Li4SiO4 pellets. It is investigated that as the increasing of liquid-to-solid ratio, the diameter of pellets gradually decreases from 1.5 mm to 0.9 mm and the interior structure becomes dense and nonporous, resulting in the inhibition of CO_2 capture capacity and the enhancement of mechanical strength. It is also found that the addition of bagasse has positive effects on promoting pellet's adsorption capacity. Meanwhile, however, it also leads to the slightly decline of mechanical strength. All of above conclusions contribute to the future development and practical applications of Li4SiO4 adsorbent pellets.

CO_2 Adsorption of Amine-Based Coconut Shell Activated Carbon: Equilibrium, Kinetics and Competitive Adsorption

Ying Ji

Zhejiang University

Email: 12127088@zju.edu.cn

The rise in atmospheric CO_2 levels results in an urgency to develop carbon capture technology. Currently, as a key of post-combustion capture technology, adsorbents such as biochar-based activated carbon have received more attention. In this work, two types of coconut shell carbons activated by KOH and NaOH are developed and investigated in terms of textural properties and adsorption/desorption temperatures, which show the best adsorption capacity of 1.52 mmol/g and complete desorption performance at 70 ℃. Due to the presence of water vapor in gas stream, which restricts the large-scale deployment of carbon capture technology, searching for the effect of H_2O of coconut shell activated carbon on CO_2 adsorption capacity is highly recommended. The optimal adsorption/desorption temperatures, humidity, and amine i.e. PEI/TEPA loading ratios of adsorbents are also determined using adsorption isotherms and adsorption rate curves.

Construction and carbon capture performance of heterogeneous catalytic system

Yuetonog Zhao

North China Electric Power University

Email: flora_369@163.com

Global energy-related carbon dioxide emissions rose by 6% in 2021 to 36.3 billion tonnes, their highest ever level, as the world economy developed. This more than offsets the 5.2 % decline caused by the COVID-19 pandemic in the previous year. Green and efficient carbon capture technology is the key to achieve carbon neutrality. The traditional chemical absorption-heating desorption strategy has a slow absorption and desorption rate during post-combustion capture. The traditional chemical absorption-heating desorption strategy has the problems of slow absorption and desorption rate, limited proton transfer and high energy consumption during post-combustion capture. Amine-based nanoparticle suspensions (nanofluids) are prepared by adding nanoparticles to alcohol-amine solutions, which can completely change the traditional CO_2 chemical absorption process by improving CO_2 capture kinetics and reducing the energy requirements of solvent regeneration. Compared with pure amine solvent, nanoparticles with catalytic effect can enhance mass transfer and improve CO_2 absorption rate and desorption rate significantly. Therefore, based on the mechanism of enhanced mass transfer and catalytic desorption of nanoparticles, this paper revealed their enhanced mass transfer behavior, clarified the reaction pathway catalyzing C-N bond fracture, and clarified the mechanism of proton transfer. The current advanced technologies and materials were summarized and introduced, and the strategies for further improvement and development were put forward, which provided new ideas for the development of carbon capture technology and had important scientific significance and application prospect for realizing the efficient utilization and green energy saving of carbon capture process of alcohol-amine system.

Enhanced CO_2/H_2 separation by GO and PVA-g-GO embedded PVAm nanocomposite membranes

Wenqi Xu

norwegian university of science and technology

email: wenqi.xu@ntnu.no

H_2 is widely recognized as the most promising non-carbon-based fuel and clean energy carrier. Currently, hydrogen is mainly obtained through steam reforming of hydrocarbons (e.g., natural gas, coal) followed by the water-gas shift reaction. A large amount of CO_2 is produced simultaneously as the process generates H_2. The technologies used in industry for the separation of CO_2 and H_2 are mainly pressure swing adsorption (PSA), cryogenic distillation, chemical absorption, and physical absorption. Compared with the methods above, the separation of CO_2 and H_2 by using membranes has the advantages of smaller footprints, lower capital cost, environmental friendliness, and simpler operation. In addition, CO_2/H_2 separation commonly uses H_2-selective membranes, which keep CO_2 in the retentate side (high-pressure side). However, it is beneficial to transportation and storage to save energy if H_2 is retained at the high-pressure side, i.e., using CO_2-selective membranes. However, the selectivity of CO_2/H_2 is usually very low since H_2 has a high diffusivity. To address the challenges, facilitated transport mechanism and 2D nanosheets has been recognized as an appropriate method to compensate the high diffusivity of H_2 by increasing solubility of CO_2. In this work, a CO_2-selective membrane based on GO- and grafting-GO-embedded polyvinylamine (PVAm)-based nanocomposite membranes are prepared and optimized for CO_2/H_2 separation. Having the highest content of primary amino groups, PVAm is wildly used in facilitated transport membranes for CO_2 separation. Incorporating GO or GO-based nanosheets in a polymeric membrane has the potential to improve the selectivity over H_2 because of its "barrier property" caused high tortuosity in membrane matrices and the additional CO_2 adsorption sites. It is worth mentioning that introducing GO or GO-based nanosheets can also increase the mechanical property of membranes under humid condition. The modified surface of the GO with higher CO_2-affinity benefits the competition of CO_2 sorption over H_2. The chemical structure, thermal stability, viscosity, and water-uptake of membrane materials, and morphology of the membranes were characterized. The effects of adding GO and PVA GO in PVAm matrix and optimal loadings of GO or PVA-GO to benefit CO_2 separation performances were determined. The CO_2/H_2 separation performances of the membranes were measured under fully humid conditions. The temperature and pressure influences of CO_2/H_2 separation were also studied.

Stabilized CO_2 capture performance of Zr-supported CaO-based sorbents synthesized by a facile and rapid combustion method

Hewen Li

Nanjing Normal University

Email: 211946002@njnu.edu.cn

Calcium looping is a promising CO_2 capture technology due to its low-cost and wide suitability. However, CaO-based sorbents easily encounter to serious sintering during high-temperature cycles, which leads to rapid loss-in-capacity for CO_2 capture. It is necessary to prepare CaO-based CO_2 capture sorbents with desirable anti-sintering capability. In this work, three synthesis methods (i.e., cellulose acetate assisted combustion, sol-gel and wet-mixing) were adopted to prepare Zr-supported, CaO-based composites. The sorbent composites prepared by cellulose acetate assisted combustion and sol-gel method possess the superior cyclic CO_2 capture performance compared to wet-mixing method. Particularly, the cellulose acetate assisted combustion method takes extremely short synthesis time, exhibiting the potential of scaled-up preparation. In addition, the optimization of calcination temperature (600 oC, 750 oC and 900 oC) and incorporation ratio of Zr-based stabilizer (5, 10, 15 and 25 wt %) for the preparation of Zr-supported, CaO-based composites by cellulose acetate assisted combustion method was conducted. Comparatively, the most suitable calcination temperature is 750 oC. The high temperature (900 oC) results in excessive sintering and lower temperature (600 oC) leads to insufficient combustion, consequently the inferior cyclic CO_2 capture performance. The Zr-supported, CaO-based composites with 25% of ZrO2 exhibit the outstanding CO_2 capture performance due to the generation of extensive CaZrO3 acting as the inert skeleton. After 17 cycles, it shows the highest CaO carbonation conversion of 63.8%, which is over 2 times that of the CaO-based sorbent without Zr-based stabilizer. Key Words: CO¬2 capture; Calcium looping; Cellulose acetate assisted combustion; Zr-supported CaO-based sorbent

Municipal solid waste pyrolysis-gasification over zeolite and eggshell supported catalysts for modification of hydrogen/carbon monoxide ratio

Dominik Horváth

University of Pannonia, Department of MOL Hydrocarbon and Coal Processing

Email: horvath.dominik@mk.uni-pannon.hu

Municipal solid waste pyrolysis-gasification over zeolite and eggshell supported catalysts for modification of hydrogen/carbon monoxide ratio Dominik Horváth, Szabina Tomasek, Norbert Miskolczi Department of MOL Hydrocarbon and Coal Processing University of Pannonia, Veszprém, Hungary e-mail: horvath.dominik@mk.uni-pannon.hu ; Abstract/Summary: The globally generated waste is growing due to the increasing population, and the development of the society. One of the aspects for long term sustainable waste utilization is the production of hydrogen and carbon-monoxide rich synthesis gas, which should be an alternative feedstock for valuable chemical production. This way looks a good option for the reduction of landfilled waste, and to mitigate the harmful effect of fossil fuel usage, which contributes the implementation of the so called circular economy. Regarding the techno-economic aspects of gasification, the hydrogen/carbon monoxide product ratio is key, because it can significantly affect the yield of syngas based products (e.g. Fischer-Tropsch hydrocarbons, methanol, energy, etc.). In this work, catalyst supported pyrolysis was carried out with various MSW feedstocks in TG-FTIR apparatus with different nickel-containing catalyst. Based on TG-FTIR results, suitable feedstocks and catalysts were chosen for the scaled-up experiments, which was carried out in tubular reactor, at two different temperatures (500°C, 900°C) in inert atmosphere using zeolite and eggshell supported Ni based catalysts. Effects of different temperatures, catalysts, feedstocks were investigated to the product yields, and gaseous product composition. In order to evaluate the effects of nickel, experiments were carried out with metal free catalyst as well. The catalysts affected not only the hydrogen/carbon monoxide ratio, but also the carbon dioxide content of the gas products.

Keywords: municipal solid waste, catalysts, syngas, tubular reactor, pyrolysis-gasification

Effects of Amine Functional Groups and Microporous Structures on CO_2 absorption performance of anion exchange resin

Xueru Wang

Xi'an Jiaotong University

Email: happywxr@163.com

Conventionally, carbon capture, utilisation and storage (CCUS) concentrates on large point-source capture of CO_2 (PSC) mostly by temperature-swing sorbents. Direct air capture (DAC) of CO_2 is rapidly emerging as a necessary complement of PSC for active removal of CO_2. DAC can deal with distributed and mobile carbon emission sources, compensate for the escape and residual emissions in the centralized point-source capture process, and not be restricted by storage sites and CO_2 transportation. This makes DAC become a promising supplementary solution of traditional CCUS. As one of the most promising materials for DAC from ambient air by moisture-swing in order to reduce greenhouse effect, amine-based anion exchange resins receive a lot of attention. In general, the absorption performance is characterized by two factors, the CO_2 absorption capacity and the absorption kinetics. It is found that the main property that determine CO_2 absorption capacity is the chemical one, i.e., the amine functional groups, while properties dominating CO_2 absorption kinetics are the physical ones, i.e., particle size, porosity and microporous structure. However, the effect of the resin's physicochemical properties on the capture performance has not been well studied. Previous studies mainly focused on the physical properties of the sorbent particles, while the chemical part receives much less attention. In this study, by testing and analyzing the absorption performance of four kinds of resins, how physical and chemical properties of the amine-based anion exchange resins affect their CO_2 absorption performances is studied systematically. After a comprehensive comparison, the order of the CO_2 absorption/desorption performance of the four kinds of resins is: macro-porous strong base resin > gelatinous strong base resin > macro-porous weak base resin > gelatinous weak base resin. Through a free energy calculation protocol by molecule dynamics and quantum chemical calculations, we studied the mechanism of the much higher absorption capacity of strong base resin compared to that of weak base resin. It is worth mentioning that the effect of the chemical property outweighs that of the physical property for moisture-swing sorbents as the performance of the gelatinous strong base resin is better than that of the macro-porous weak base resin. Through further analysis we conclude that the most superior sorbent is the macro-porous strong base resin due to its strong amine groups and large inner pore sizes. The present study provides a screening criterion for selecting suitable materials for DAC of CO_2 and shows a way of preparing better absorbents for enhancing capture performance.

Preparation and chemical chain combustion performance of doped Fe2-XTMXO3 oxygen carrier

Liangliang Meng

Ningxia University

Email: 2477435426@qq.com

Chemical chain combustion (CLC) is a new type of energy efficient utilization technology, which decouples the traditional reaction into two gas-solid reactions with the help of oxygen carriers, so as to realize the directional conversion of energy and the low-consumption separation of products. Fe2O3 has the problem of low reactivity as an oxygen carrier. A series of transition metal-doped iron-based oxygen carriers were designed and prepared, and the reaction mechanism and performance regulation were studied based on the complementary and synergistic effects between bimetals. Iron-based oxygen carriers doped with Mn, Co, Ni, Cu, and Zn were prepared by co-precipitation method, and XRD, SEM, and XPS characterizations proved that transition metals were successfully doped and uniformly distributed. H_2-TPR test showed that transition metals were successfully doped. Doping can improve the activity and copper doping has the best activity. Finally, the TGA properties of iron-based oxygen carriers under 10% H_2 atmosphere at 550, 600, 650, 700, and 750℃ were studied. We found that the iron base undergoes a phase transition from Fe2O3-Fe3O4-FeO-Fe. Through the study of the overall and staged apparent activation energy and pre-exponential factor, we found that the shrinking core model (ball) under 3% doping was in good agreement with the overall, and concluded that Co (40.5), Ni (41.0), Cu The doping of (40.1) is better than that of Mn (54.8) and Zn (48.7kJ/mol). In our staged study on Co, Ni, Cu, and doped iron-based oxygen carriers, we found that the activation energy of Fe2O3-Fe3O4 stage is about 20-30 kJ/mol, and the activation energy of Fe3O4-FeO stage is about 40-50 kJ/mol mol, the activation energy of FeO-Fe stage is about 60-80 kJ/mol, which can well explain that the lattice oxygen of Fe2O3-Fe3O4-FeO is mainly used in the chemical chain process. This research is of great significance for realizing the intensification of coal chemical chain combustion process and cleaner production.

In-situ Polymerization of cobalt porphyrin on carbon nanotubes for efficient electrochemical CO_2 reduction

Shengshen Gu, Academic

Changzhou University

Email: gushengshen@126.com

Cobalt porphyrin based catalysts have drawn wide attention for application in CO_2 electrochemical reduction reaction (CO_2ERR) as they are robust, efficient and noble metal free. Herein, an innovative technique was employed for immobilization of cobalt tetra(4-ethynylphenyl)porphyrin (CoTEP) onto carbon nanotubes (CNTs). The approach is based on the formation of a covalent porphyrin framework by chemical polymerization via Hay coupling reaction. The hybrid material (CoTEP@CNTs) exhibited enhanced activity towards CO_2-to-CO electroreduction. CoTEP@CNTs showed a specific Faradaic efficiency (FE) of 90 % and turnover frequency (TOF) of 2.1 s-1 at the overpotential of 570 mV. Compared to the physically mixed catalyst (CoTEP/CNTs), CoTEP@CNTs improved FE by 10 % and TOF by a factor of 1.3. The improvement in the performance was also observed in the long run electrocatalysis. To the best of our knowledge, this is one of the best polymerized porphyrins for CO_2ERR. Characterizations reveal that the polymerization of CoTEP on CNTs led to a more uniform layer of porphyrin molecules on the sidewalls of CNTs and, as a result, contributed to the enhanced efficiency of the catalyst. To conclude, the uniform layer of porphyrins achieved by polymerization is promising in enhancing the performance of electrocatalysts towards CO_2ERR.

ReaxFF study on CLC behavior of N-PACs with different N microchemical environments in CuO oxygen carriers

Chang Geng

State Key Laboratory of High-Efficiency Utilization of Coal and Green Chemical Engineering ,College of Chemistry and Chemical Engineering, Ning xia University

Email: gengchang1111@163.com

Using first-principles molecular dynamics (MD) simulations of ReaxFF , the effects of different temperatures on oxygen release and main product formation in three N-PACs models were analyzed, and the influencing factors of temperature on product release and the primary and secondary paths of product formation were analyzed. The migration paths of fuel molecules in CLC under different N environments were studied, and a three-stage thermal reaction network system of N5/N6/NQ was established. Finally, through the analysis of oxygen release mechanism of oxygen carrier, the differences of combustion phenomena of different systems are further explained, three oxygen release pathways and four oxygen release stages of CuO oxygen carrier were demonstrated, the reaction kinetics of three chemical chain combustion processes are simply evaluated.

Analysis of the energy structure of a typical paper industry in northern China

Yuying Huang

Shandong Jianzhu University

Email: yuying_huang2020@163.com

At present, the paper industry, as an important raw material base industry, has always been dominated by coal in its energy structure, with the sum of coal and electricity accounting for more than 80% of total energy consumption. Although it accounts for a relatively low share of total carbon emissions, the continued expansion of the industry has led to rising energy demand, which, combined with the current high-carbon energy structure dominated by coal, has made it necessary for the paper industry to take stronger carbon reduction measures in implementing the national "double carbon" target requirements. Therefore, the quantification of the energy and carbon intensity of the paper industry and the acceleration of the transformation of the energy structure have become the focus of current research. Methods This study analyses the production data of three paper companies (WD, TY and HY) with different energy mixes, combining information on carbon emissions, product output, carbon emissions per unit of product and energy consumption costs per unit of product in the paper industry in a variety of dimensions. The analysis includes direct emissions from fossil fuel combustion, indirect emissions from fossil fuels, electricity and heat, as well as a full process analysis of carbon emissions from fossil fuels, electricity, heat and waste water treatment. Conclusions According to the results of CO_2 emission intensity per unit and energy CO_2 emission ratio, it can be seen that natural gas accounts for the largest proportion in the direct emission process; the indirect emission process with a high proportion of electricity has low CO_2 emission per unit product, and the proportion of electricity in the energy of paper enterprises should be increased appropriately; aerobic treatment of wastewater accounts for only 0.2% in the whole process, but its greenhouse effect cannot be ignored. Based on the carbon emissions per unit product and the energy consumption cost per unit product, it can be found that WD has the highest carbon emissions and the highest consumption cost at the same time, indicating that the coal-based energy structure has a higher carbon emission intensity and cost, while the natural gas-based energy structure is relatively low, which is more in line with the dual carbon policy and the requirements of industrial green development. Keywords:paper industry; carbon accounting; carbon assessment; energy-resource structure Acknowledgment This study was supported by the National science foundation of Shandong Province (No. ZR2020ME236), National key research and development program (2022YFE0105800), Research and development project of the Ministry of housing and urban rural development (K20210424), Science Foundation of Shandong Jianzhu University Grant (No. XNBS1824). Reference [1] Chen Xian Yue. Challenges and coping strategies for the paper industry under the "double carbon" target[J]. China Paper,2021,42(19):10-13+7. [2]Ye Yucheng, Yan Weilin. Current situation of energy

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Analysis of carbon capture from a coal-fired power plant integrating heat pump technology

Liu Wei

Institute of Refrigeration and Cryogenics, Zhejiang University

Email: 12027057@zju.edu.cn

Carbon Capture and Storage (CCS) is considered as a promising technology to mitigate global warming. However, adsorption technology, especially temperature swing adsorption (TSA), requires large energy consumption in the regeneration process, which would increase operation cost of carbon capture unit. Here, an absorption heat pump is introduced into carbon capture system which aims to supply high-level regeneration heat using waste heat sources from coal-fired power plant. Temperature difference between absorption temperature of heat pump and regeneration temperature of carbon capture system is ignored. Results indicate that when generation, evaporation, condensation temperature of heat pump are 80℃, 80℃ and 20℃, adsorption and regeneration temperature are 25℃ and 135℃, respectively, Coefficient of Performance (COP) of heat pump can reach 0.362, purity and recovery of TSA process are 85.2% and 72.8%, respectively. When regeneration temperature decreases from 135℃ to 120℃, COP increases to 0.370, but purity and recovery decreases to 82.0% and 58.2% respectively. The integration of heat pump into carbon capture system would have great potential in field of energy-saving and carbon-mitigation.

Synthesis of a novel copper silicon molecular sieve for CO_2/N_2 separation

Nan Li

State Environmental Protection Key Laboratory of Eco-Industry, Northeastern University, China

Email: 414612576@qq.com

Since the Industrial Revolution, the massive consumption of fossil fuels, as well as a series of man-made activities, have emitted large amounts of carbon dioxide (CO_2) into the atmosphere, resulting in climate problems such as global warming. Pressure swing adsorption (PSA) is the most promising technology in the field of CO_2 separation. Adsorbent is the core of PSA technology. Efforts to curtail the increase in atmospheric CO_2 concentration rely on the development of adsorbents that capture CO_2 with high selectivity and low cost. Here, we report a novel type of copper silica molecular sieve that was prepared by hydrothermal synthesis method with sodium silicate as silicon source and copper sulfate as copper source. The effects of different synthesis conditions on the new copper silicon molecular sieve were discussed. Finally, the synthesis method with the best crystallinity of the new copper silicon molecular sieve was obtained. The synthesized samples were characterized. The synthesized samples had new XRD patterns, good crystallinity, complete skeleton structure and good thermal stability. These results showed that a new type of copper silicon molecular sieve was successfully synthesized. The CO_2 and N_2 adsorption data of the new copper silicon molecular sieve were fitted well with the Toth isotherm model. The CO_2/N_2 separation performance of the new sample was tested, and the selection factors were calculated. The calculation results indicated that the selection factors were greater than 5, which proved that the new copper silicon molecular sieve had high adsorption selectivity. This new material can be well applied to the separation of CO_2 and N_2. This result provides a new prospect for the design of copper silicon molecular sieves with high adsorption efficiency.

Process design of hydrogen-enriched gas production through two-stage sorption-enhanced biomass gasification

Godknows Dziva

Tianjin University

Email: godknowsdziva@tju.edu.cn

Green hydrogen and bioenergy with carbon capture are expected to play an important role in the transition to net-zero emissions. This study presents a novel process for producing hydrogen-enriched gas through sorption-enhanced gasification(SEG) of biomass. SEG is a process that integrates decoupled gasification and calcium looping carbon capture to convert solid fuels into hydrogen-rich syngas. Traditionally, SEG uses dual fluidized bed gasification to produce ~75% H_2(dry basis). Independent, catalyzed post-gasification reforming is often used to further enrich the hydrogen concentration. This study proposes an integrated two-stage SEG process that employs a fluidized bed gasifier and a counter-current moving bed reformer to yield over 95% H_2(dry basis). The first stage involves typical high-temperature sorption-enhanced gasification in a fluidized bed. Then the product gas from the first stage undergoes simultaneous sorption-enhanced reforming of CO, CH4 and tar at relatively lower temperatures. Exothermic carbonation and water-gas shift provide heat for endothermic steam reforming, thus creating an autothermal process. This study employs a model based on Gibbs free energy minimization to assess the thermodynamic properties of the autothermal moving bed reformer. The effect of calcium looping ratio, steam-to-carbon ratio and feed temperatures on the product gas distribution and bed temperature profiles is analyzed to establish optimal operating conditions. Sorbent regeneration with oxy-combustion utilized in this design can achieve net removal of carbon when the CO_2 captured is sequestered or further utilized. The potential integration of the proposed process in abating CO_2 emissions from various carbon-intensive industries is discussed. In addition, technical challenges related to bed material particle size and circulation are qualitatively examined.

Hydrotalcite derived NiFe alloys anchored on periclase-phase (Mg, Al)Ox nanosheets for CO_2 reforming of toluene assisted by DBD plasma

Dai Jing

Nankai University

Email: daijing@mail.nankai.edu.cn

The removal of tar and CO_2 in syngas from biomass gasification is crucial for the upgrading and utilization of syngas. CO_2 reforming of tar is a potential solution by simultaneously converting the undesirable tar and CO_2 to syngas. In this study, a hybrid dielectric barrier discharge (DBD) plasma-catalysis system was developed for the CO_2 reforming of toluene (CRT), as a model tar compound, at low temperature (200 oC) and ambient pressure. Periclase-phase (Mg, Al)Ox nanosheet supported NiFe alloy catalysts with various Ni/Fe ratios were synthesized from ultrathin Ni-Fe-Mg-Al hydrotalcite precursors and employed in the plasma-catalytic CRT reaction. The result demonstrated that the plasma-catalysis system is promising in promoting the low-temperature CRT reaction by generating a synergy between DBD plasma and catalyst.

Functionalized two-dimensional g-C3N4 nanosheets in PIM-1 mixed matrix membranes for gas separation

Hui Shen LAU

Xiamen University Malaysia

Email: mce2009001@xmu.edu.my

Two-dimensional (2D) nanosheets have drawn much fascination as nanofillers for membrane gas separation. Taking the advantages of high surface-to-volume ratio, large specific area and tunable surface functionality, the incorporation of these sheet-like fillers into mixed matrix membranes (MMMs) only at a mere loading offers the opportunity for a breakthrough in separation performance. Graphitic carbon nitride (g-C3N4) is a cost-effective 2D nanomaterial that has the most stable carbon nitride allotrope at ambient pressure and temperature. Inherent and periodic triangular ultramicropores are formed throughout the g-C3N4 planar structure that favors precise sieving of gases with small kinetic diameter. Our endeavor in this study is to introduce functional groups onto the g-C3N4 nanosheets and incorporated them as fillers to prepare MMMs for gas separation. The effect of functionalization is evaluated based on four types of functional groups, namely sulfuric acid, aliphatic amino, aromatic amino, and sulfonic groups. The modified fillers are incorporated into PIM-1 polymer matrix and the separation performance is examined. To our surprise, the sulfonic acid functionalized g-C3N4 MMMs showed no apparent defects or agglomeration of particles even at a loading of 10 wt%, suggesting the good compatibility between the fillers and polymer matrix. With a mere loading of 1 wt%, the resultant MMMs exhibited H_2, CO_2, and N_2 permeabilities of 2018, 3740, and 189 Barrer, respectively, along with CO_2/N_2 and H_2/N_2 selectivities enhancement up to 19% and 15%. Credited to the periodic ultramicropores in g-C3N4, the MMMs with 5 wt% fillers surpassed the 2008 Robeson bound for H_2/N_2 and $O2/N_2$. Remarkably, these findings signify the great potential of sulfonated g-C3N4 MMMs for hydrogen purification, air separation and CO_2 capture.

Fabrication of incineration bottom ash-derived CaO-based sorbent with self-enhanced CO_2 capture capacity and stability

Zhang Zhikun, Academic

Hebei University of Technology

Email: zhangzk@hebut.edu.cn

CO_2 capture using CaO-based sorbent is a promising and effective CO_2 mitigation strategy due to its high theoretical capacity of CO_2 adsorption and potential use in large scale. The preparation of waste-derived CaO-based sorbents for CO_2 capture has received great interests due to its economic feasibility via waste recycling. In this work, the development of a novel self-enhanced CaO-based sorbent via the entire utilization of municipal solid waste incineration bottom ash (BA) is reported. Specifically, CaO was extracted from BA while the residues were added back to the extracted CaO after thermal passivation, which severed as an inert stabilizer to improve the CO_2 capture capacity and sintering resistance of CaO. The effects of BA residue-derived stabilizer (BAS) additive amount and carbonation temperature on the CO_2 capture performance were studied. The results demonstrated that the CO_2 capture capacity exhibited a volcano-type variation with the increase of both BAS additive amount and carbonation temperature. The BAS(20wt.%)/CaO sorbent (BAS/CaO=20/80) exhibited the most superior CO_2 capture capacity of 0.15 g/g after 10 cycles of cyclic CO_2 adsorption and desorption due to that wet mixing increases the adsorption capacity by increasing the pore size of the adsorbent. Thermal modification transforms the crystalline SiO2 in the inert stabilizer into highly reactive amorphous SiO2 . The reaction between amorphous SiO2 reacts with CaO to form Ca2SiO4, while the amorphous Al2O3 in the inert stabiliser reacts with CaO to form Ca12Al14O33. These two substances have good anti-sintering and support properties, thus improving the cyclic stability of CaO. This study provides a promising method to achieve a cost-effective CO_2 capture candidate with self-enhanced capacity by completely reusing solid wastes, which eliminates the treatment and disposal of secondary residues that was rarely considered in previous studies.

Comparative life cycle assessment on metal-organic frameworks production for CO_2 capture

Siew Kei Lau

Xiamen University Malaysia

Email: MCE2104002@xmu.edu.my

Global warming has undoubtedly been the trending topic in this era, with greenhouse gases, particularly CO_2, being its main cause. Scientists and governments are proactively searching for strategies to reduce the emission of greenhouse gases. Metal-organic frameworks (MOFs) consist of metal ions and organic ligands in a coordinated network. Among all MOFs, zeolitic imidazolate framework-8 (ZIF-8) has emerged as a promising contender for CO_2 capture. The life cycle assessment (LCA) of various ZIF-8 production processes was investigated, including solvothermal (DMF), solvothermal (MeOH), microwave, sonochemical, mechanochemical, and dry-gel conversion. The results revealed that among the 18 categories of evaluation studies, marine ecotoxicity is the most affected, followed by human non-carcinogenic toxicity and terrestrial ecotoxicity. Except for the solvothermal (MeOH) approach, the solvent for washing, N, N-dimethylformamide (DMF), was the leading factor in environmental deterioration. In comparison to the solvothermal (DMF) method, replacing the DMF solvent with methanol (i.e., solvothermal (MeOH) method) greatly reduced the impact on human health, ecosystem, and resources. The mechanochemical technique has the lowest overall environmental effect due to its fewer production processes and ease of operation. As a result, this study examines the environmental effects of several ZIF-8 synthesis processes to accomplish long-term production and ultimately minimize global warming.

Study on synthesis catalyst of municipal Solid waste incineration bottom ash for dry reforming of methane

yuqi zhang

Hebei University of Technology

Email: zhangyuqiqi123@126.com

The municipal waste incineration bottom ash is used as the raw material of the catalyst carrier. Calcium acetate was extracted with acetic acid, and calcium acetate was used as the precursor of CaO accelerator. The remaining ash was used as the catalyst carrier, and metal nickel was supported by sol-gel method. The catalytic performance of catalysts with different CaO contents in methane dry reforming was discussed. With a flow rate of 30ml/L, a reaction temperature of 900℃, and the presence of Ni/MA(M)-20Ca catalyst, the conversion rates of methane and carbon dioxide can reach 83.11% and 91.51%, and the reaction has excellent stability. This will provide a method to fully utilize municipal waste incineration bottom ash in methane dry reforming and conduct more research.

Modelling the technoeconomic and life cycle assessment of the bioenergy carbon capture and storage (BECCS) in Southeast Asia

Joni Jupesta,Academic

Research Institute of Innovative Technology for the Earth (RITE)

Email: jjupesta@rite.or.jp

The 6th Intergovernmental Panel on Climate Change (IPCC) Assessment Report has mentioned that carbon dioxide removal (CDR) technologies have potential to remove CO_2 from the atmosphere. There is high potential of bioenergy from biomass residues, mill effluent and palm oil products to support net zero emissions in form of bioenergy with carbon capture and storage (BECCS). BECCS is the most mature of all the carbon dioxide removal technologies, as both bioenergy production and carbon capture and storage (CCS) have been separately proven at commercial scale. Oil palm biomass residues, namely, empty fruit bunches, mesocarp fiber, frond, trunk, and palm kernel shell, are abundant in Southeast Asia countries, especially in Indonesia, Malaysia, and Thailand. These residues could be processed into various forms: pellet biomass, biochar, and syngas, while the mill effluents can be processed into biomethane, and the palm oil could be processed into biodiesel fuel. In this study we conduct spatial analysis, technoeconomic analysis (TEA) and life cycle assessment (LCA) to quantify the energy, economic and environmental impacts of the BECCS from palm oil. The spatial analysis will be conducted by using ArcGis 10.8, TEA will be conducted by using R software and the LCA will be conducted by using SImapro 9.3 software as tools. Two scenarios will be analyzed: bioenergy with and without CCS. It is expected that the study could give information to relevant stakeholders on the potential of BECCS in Southeast region as one of the CDR technologies.

Computational catalyst design for solvent regeneration in post-combustion CO_2 capture (PCC) process

Muhammad Ibrahim Irshad

University of Hull

Email: m.irshad-2021@hull.ac.uk

Global warming is attributed to anthropogenic carbon dioxide (CO_2) emissions. To achieve net-zero carbon emission and mitigate global warming, it is paramount to capture and store CO_2 released from large industrial processes. Post-combustion carbon capture (PCC) using chemical absorption with solvents like monoethanolamine (MEA) has proven to be the best option to capture CO_2 from large stationary sources [1]. However, one of the key challenges with PCC by chemical absorption is the energy consumption in the solvent regeneration which leads to a high cost of capture and energy penalty on the host plant [2]. This issue can be addressed by catalysts-aided solvent regeneration. The concept of catalysts-aided regeneration has been proven and different catalysts such as γ-Al2O3 and HZSM-5 have been evaluated for single amine and blended amine solvents including MEA, MEA-DEAB and MEA-MDEA [3]. The studies [4] have shown up to 40% regeneration energy and regeneration temperature below 100oC as opposed to at least 120oC in uncatalysed cases. However, the kinetics of the catalysed reactions have barely been reported and this limits more expansive investigation of the process level performance through modelling and simulation. In this study, a methodology via computational chemistry calculations involving density functional theory (DFT) modelling is proposed for obtaining the transition states for different catalytic reactions. This can be used to determine the energy barrier and other kinetic parameters. A preliminary result has been obtained for single catalysts such as γ-Al2O3, HZSM-5, V2O5, MoO3 and composite catalysts such as Ce(SO4)2/ZrO2. The obtained energy barriers were shown to be consistent with reported results in the literature. Our proposed approach can be applied to identify missing kinetic information in catalyst-aided regeneration and will therefore benefit model development for PCC systems with catalyst-aided regeneration. Acknowledgement This project has been funded under the Engineering and Physical Science Research (ESPRC)/UK carbon Capture and Storage Research Center (UKCCSRC) Flexible funding 2021 (REF:EP/P026214/1) Reference 1. Liao, P., Li, Y., Wu, X., Wang, M. and Oko, E. 2020. Flexible operation of large-scale coal-fired power plant integrated with solvent-based post-combustion CO_2 capture based on neural network inverse control. International Journal of Greenhouse Gas Control 95; 102985. 2. Lai, Q., Toan, S., Assiri, M. A., Cheng, H., Russell, A. G., Adidharma, H., Radosz, M., Fan, M. 2018. Catalyst-TiO(OH)2 could drastically reduce the energy consumption of CO_2 capture. Nat. Commun. 9(1); 2672. 3. Shi, H., Naami, A., Idem, R. and Tontiwachwuthikul, P. 2014. Catalytic and non-catalytic solvent regeneration during absorption-based CO_2 capture with single and blended reactive amine solvents. International Journal of Greenhouse Gas Control 26; 39-50 4. Zhang, X., Fu, K., Liang, Z., Yang, Z., Rongwong, W. and Na, Y. 2014. Experimental studies of regeneration heat duty for CO_2

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Novel Tungsten doped Iron Oxide as an oxygen carrier for Chemical Looping Combustion

Srigan N. Moharir

(MSc- Advanced Chemical Engineering Postgraduate Student, Imperial College London)

Jose J Morales Corona

(PhD Student, Department of Chemical Engineering, Imperial College London)

Dr. Paul S. Fennell

(Professor, Department of Chemical Engineering, Imperial College London)

Email: srigan.moharir21@imperial.ac.uk

With a high energy conversion efficiency, 'Chemical Looping Combustion (CLC) Technology' can certainly be designated as a favourable carbonaceous fuel conversion technology with an inherent CO_2 capturing ability. Chemical Looping Combustion directly falls under the umbrella of Carbon Capture Science and Technology. In the past few decades, the capability of Chemical Looping Combustion Technology to obtain high purity gas products has been of great interest to researchers across the globe. Oxygen carriers form an integral part of the Chemical Looping Combustion Technology. Oxygen carriers facilitate the transfer of oxygen to the reactors. Metal oxides are known to play a vital role in the Chemical Looping Combustion Redox reactions. During the reduction phase, the amount of oxygen ions necessary for the hydrocarbon conversion of CO_2 and H_2O is donated by oxygen carriers. On the other hand, during the oxidation phase, oxygen carriers in the form of depleted metal oxides are provided with oxygen from the air and the overall reaction results in the production of heat and energy. The potential of mixed oxides as oxygen carriers in the chemical looping process has been an interesting aspect of CLC research, as it significantly expands the design space for primary oxide selection and numerous related applications. Metal oxides like Fe2O3 are known to have high tunability in terms of their bulk thermodynamic, surface and structural properties. These properties can prove to be of great importance towards the rationalization of the design of new Fe2O3 based oxygen carriers for numerous Chemical Looping applications. For the scope of this work, iron oxide was chosen as the base metal oxide due to its explicit properties of low cost and being environmental-friendly. Another reason why naturally occurring ores are suitable as oxygen carriers in the CLC process is because of their relative abundance which makes them viable to be used extensively for the scope of this project. This work demonstrates the benefits of doping Tungsten (W) within the Fe2O3 matrix and thus producing a completely new oxygen carrier. The oxygen carrier was synthesized via Wet-Impregnation and Quantitative Wet-Impregnation methods whilst using different compositions of the amount of Tungsten being doped. To assess the performance of this W-doped oxygen carrier, a thermogravimetric analyser was used. Whereas, to understand various physical and chemical properties of the material, characterisation techniques like XRD, XRF, SEM, BET crushing strength etc. were employed. The results indicated that doping tungsten in iron oxide as an oxygen carrier

is relatively stable and worked considerably well during the redox cycles without any agglomeration and sintering. Tungsten impregnated iron oxide-based oxygen carriers showed good mechanical resistance and enhanced surface properties. The density of the newly formed oxygen carrier showed a slight reduction in bulk density as compared to the iron oxide thus, helping it to achieve better fluidisation. Finally, this doping of tungsten in iron oxide has improved the performance of this novel oxygen carrier without any reduction in the oxygen-carrying capacity. Since there is almost no evidence in the literature record regarding iron oxide-based oxygen carriers doped with tungsten, the findings from this project will certainly be unique and will contribute significantly to the existing literature on numerous mixed metal oxide oxygen carriers."

Dry reforming of methane by LaNiO3 perovskite oxide: influence of preparation methods and research on regeneration properties

Dingshan Cao

State Key Laboratory of Coal Combustion, School of Energy and Power Engineering, Huazhong University of Science and Technology

Email: cao_ds@hust.edu.cn

The dry reforming of methane (DRM) process has attracted much attention in recent years for the direct conversion of methane and carbon dioxide into high value-added syngas. The catalysts with perovskite oxides as precursors showed good reaction performance and stability. In this study, LaNiO3 was prepared by sol-gel method, coprecipitation method, hydrothermal method and solid phase method to study the influence of preparation methods on the catalyst structure and DRM reaction performance. The regeneration properties of the used LaNiO3 catalyst was also investigated with steam, CO_2 and air as regeneration atmosphere, respectively. The results showed that LaNiO3 prepared by sol-gel method formed a more uniform perovskite phase and had better initial DRM performance. The regeneration tests showed that three kinds of gasification agents could remove the carbon deposited on the catalyst surface after reaction, and air atmosphere had the best regeneration property. In addition, LaNiO3 was found to have a high-temperature activation phenomenon in DRM. In DRM reaction at 750 °C, the CH4 and CO_2 conversion rate of the sample regenerated by air after high-temperature (850 °C) DRM reaction was 25% and 17% higher than that of fresh sample, respectively. TEM images showed that the active sites of the sample regenerated after high-temperature reaction were more likely to be exposed in the reaction atmosphere. Further tests showed that the carbon deposition rate of LaNiO3 in DRM reaction increased with the increase of reaction duration due to the gradual loss of lattice oxygen. The lost lattice oxygen could be replenished by the regeneration step.

Carbon Capture and Utilization in Low-Carbon Cements: Impact of Precipitated Calcium Carbonate on the Rheology of Portland Cement Blends

Rukayat Oyiza Salawu

The University of Aberdeen

Email: r01rs22@abdn.ac.uk

One of the world's biggest industries emitting anthropogenic CO_2 is the cement plant. In other to mitigate the emissions ground calcium carbonate (CaCO3) is used as an additive in Ordinary Portland cement and the industry has had a reduction in the CO_2 emissions with the use of ground-CaCO3. However, ground-CaCO3 is carbon positive. this which is branded as Portland cement. Carbon Capture and Utilization (CCU) processes can be used to tackle the phenomenon of climate change and create valuable products that can be used by several sectors. Precipitated calcium carbonate (PCC) is a form of calcium carbonate that can be manufactured through CCU. This study examines the rheological properties of cement blends with additives (different PCC types) in different ratios and quantities. Nano-calcite, Aragonite in powder forms and scalenohedral in crystalline consistency were the PCC tested at 5%, 7%, 10% and 15% at 0.47, 0.50, 0.53 water/solids (w/s) ratio. the cement type which was used for all samples is CEM I 52.5N OPC by Hanson Cement UK. Cement type I is classified in strength classes according to a strength test which is performed after 28 days of curing. The weakest structure identified at the highest w/s ratio in contrast to strongest structures which were spotted at lowest w/s ratio. The strongest structures from the tested pastes appeared at the lowest w/s ratio with the highest percentages of additive. As the proportion of additive and the ratio changed, the yield stress (τ_y), the plastic viscosity (μ_p) and the workability of the pastes, were affected. Scalenohedral formed the weakest, aragonite formed stronger while nano-calcite formed the strongest pastes, these were compared to the ground-CaCO3 cement pastes. The porosity of the paste also had an impact on the strength of the pastes, since at the highest quantities of additives, the pastes became stronger. The strongest paste of scalenohedral had, τ_y smaller by 22.9%, μ_p higher by 15.9% and had similar workability to the ground-CaCO3 cement paste. The strongest paste of aragonite had τ_y higher by 9.8%, μ_p higher by 4.8% but it had smaller workability. The strongest paste of nano-calcite had τ_y greater by 41.1%, μ_p smaller by 9.1% while it had the smallest workability. As the surface area of the cement pastes increased, the strength of the paste increased.

Study of water-lean solvents for the post-combustion CO_2 capture process

Eni Oko, Academic

Newcastle University

Email: eni.oko@newcastle.ac.uk

Carbon capture from stationary sources such as power plants is required to cost-effectively reach net-zero emissions and mitigate climate change. Solvent-based post-combustion CO_2 capture is the most established technology option for implementing carbon capture. However, the water concentration in existing solvent blends is over 70% and due to the high heat capacity of water, the energy requirement for regenerating the solvents and the regeneration temperature is high, typically up to 4 GJ/tCO_2 and over 120oC respectively, leading to high capture cost (>£37/ton CO_2) and >10% energy penalty on the host power plant (Oko et al. 2017). One way to address this problem is to identify and develop new solvent blends that use reduced water concentration, so-called water-lean or non-aqueous solvent. The most popular water-lean solvents reported for PCC application use an alcohol base such as propanol in place of water and are promising in lowering both the energy consumption and the regeneration temperature (Barzagli et al. 2014). There are however no reported models of the PCC process using a water-lean solvent that can be used for a more systematic assessment of the process. This study offers a detailed review of reported water-lean solvents undertaken via option appraisal to identify the most matured water-lean solvent blends and systematically compare their performance. An example water-lean solvent, namely AMP-EG/PrOH is selected and further investigated through modelling and simulation. The model is obtained via rate-based modelling in Aspen Plus for the absorber and desorber units and used to perform a comparative performance evaluation against aqueous AMP solvent. Acknowledgement The authors are grateful for the contributions and support from UNIPER, UK Engineering and Physical Science Research (EPSRC), and the UK Carbon Capture and Storage Research Centre (UKCCSRC) for funding this project (REF: EP/P026214/1) Reference Barzagli, F., Lai, S. and Mani, F. 2014. Novel non-aqueous amine solvents for reversible CO_2 capture. Energy Procedia 63, 1795-1804. Oko, E., Wang, Meihong. And Joel, A.S. 2017. Current status and future development of solvent-based carbon capture. International Journal of Coal Science and Technology 4, 5-14.

Modelling and Analysis of Catalysts-aided Solvent Regeneration in Post-Combustion CO_2 Capture Process

John Olusoji Owolabi

University of Hull

Email: get2owolabijohn@gmail.com

Post-combustion CO_2 capture with solvent is the most matured option for implementing CO_2 capture technology. However, this technology requires high amount of energy to regenerate the solvent, typically over 4 GJ/tCO_2 for the conventional monoethanolamine (MEA) solvent which impacts the cost per tCO_2 and the energy penalty on the host power plant (Alivand, Mazaheri et al. 2020). Catalyst-aided solvent regeneration has been identified to have the potential to substantially reduce the thermal energy requirement in solvent regeneration in the technology. There is however limited process level analysis that demonstrates the performance of catalysts-aided regeneration as majority of existing studies are focused on the catalyst characterisation and testing. This study will address this limitation by providing a detailed model of the post-combustion CO_2 capture process with catalyst-aided solvent regeneration. The model, based on the HZSM-5 catalyst and MEA solvent, will be obtained through rate-based modelling in Aspen Plus with catalyst-aide regeneration implemented as a custom model in Aspen Custom Modeller. This model will be validated and used to determine the cyclic loading performance, solvent regeneration energy and temperature. More also, the techno-economic analysis will be comprehensively carried out to determine the cost implications of this process.

Biocatalytic composite membranes for CO_2 capture

Cristhian Molina Fernández

UCLouvain

Email: cristhian.molina@uclouvain.be

Nature has developed very active and specific catalysts that are critical for living organisms' existence. The application of some of such biocatalysts in CO_2 capture and utilization has recently attracted large interest from the research community and the industry. For example, they have been applied to CO_2 absorption aiming to reduce the liquid side mass transfer resistance. This resistance is dominating the overall mass transfer and it can be reduced by catalyzing the slow CO_2 hydration reaction. Besides, they have also been incorporated in selective membranes. These membranes usually displayed improved permeability and selectivity due to the facilitated transport mechanism [2]. In addition, these biocatalysts are usually immobilized in/on a carrier to protect them from the harsh conditions in CO_2 capture and ensure long-term stability. Depending on the immobilization method, the immobilization results in different degrees of stabilization and activity loss. We report here the fabrication and characterization of novel composite membranes with immobilized biocatalyst for CO_2 bioconversion. These membranes were prepared by a novel method that ensured a good and straightforward biocatalyst immobilization. The membranes were structurally characterized by SEM while their activity in different conditions was evaluated using p-NPA hydrolysis. In addition, to demonstrate their applicability, the biocatalytic composite membranes were tested in a gas absorption set-up showing an increase in the overall mass transfer coefficient with respect to the pristine support. These membranes could also be interesting for other applications as the combination of a selective barrier and the biocatalyst leads to process intensification (reaction + separation in the same device).

Multiphase reacting flow modeling of MEA-based CO_2 absorption in packed columns

Yash Girish Shah

National Energy Technology Laboratory; Leidos Research Support Team (LRST); Leidos

Email: yashgirish.shah@netl.doe.gov

Carbon capture and storage (CCS) systems are one of the potential technologies for reducing global atmospheric CO_2 levels. Among the currently available CCS technologies, chemical absorption has been proposed as a viable strategy for reducing carbon emissions from point sources, such as flue gases emitted from carbonaceous combustion[1], or directly from air. While the technological basis for such solvent-based packed absorption columns has existed for several decades, the optimization of such devices for increased absorption performance and economic constraints remains a challenge. This is partly because of the lack of understanding of the complex nonlinear coupling between flow hydrodynamics and geometrical features of the packing, thermodynamics, and chemistry of the absorption process. To facilitate this understanding, recent studies have provided insights into the complex hydrodynamics within packed columns by identifying the parameters that affect liquid holdup and interfacial area using computational fluid dynamics (CFD) simulations [2,3]. However, obtaining a fuller understanding of the key geometrical and thermophysical parameters that affect the chemical absorption process requires incorporation of the coupled solvent reaction kinetics and thermodynamics. In this work, we aim to extend the current understanding of the absorption process by developing a numerical framework that is capable of simulating the coupled dynamical interactions between column hydrodynamics, thermodynamics, and chemical reactions for columns with structured packing. More specifically, we develop a two-phase CFD model for chemical absorption in monoethanolamine (MEA), wherein the reaction kinetics, temperature, and composition dependent thermophysical properties of the MEA–H_2O–CO_2 system are incorporated from the Institute for Design of Advanced Energy Systems (IDAES) framework [4] under the Carbon Capture Simulation for Industry Impact (CCSI2) initiative. We model the two phases as multi-component immiscible reacting mixtures of MEA–H_2O–CO_2 solution and flue gas and numerically solve the transport equations for participating species separately within each phase using ANSYS Fluent. We explicitly track the interface using a volume of fluid method [5] and quantify the chemical absorption using a six-species, two-reaction chemical mechanism [4]. We demonstrate the applicability of the proposed model by quantifying CO_2 absorption characteristics for reference packing geometries. References: 1. Plaza, Jorge Mario. "Modeling of carbon dioxide absorption using aqueous monoethanolamine, piperazine and promoted potassium carbonate." PhD diss., 2012. 2. Fu, Yucheng, Jie Bao, Rajesh Kumar Singh, Richard Feng Zheng, Christine M. Anderson-Cook, K. Sham Bhat, and Zhijie Xu. "The influence of random packed column parameters on the liquid holdup and interfacial area." AIChE Journal (2022): e17691. 3. Fu, Yucheng, Jie Bao, Rajesh Singh, Chao Wang, and Zhijie

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Experimental study on the absorption and desorption of CO_2 in the exhaust gas of ships by Cu-Al2O3 nanofluids

Kong Cunjin

Chongqing Jiaotong University

Email: 915198692@qq.com

The most widely used CO_2 capture method is organic amine absorption. However, the method still has a bottleneck that is difficult to overcome, that is, how to increase the gas-liquid mass transfer rate.Based on nanofluids, experiments have shown that adding nanoparticles to the base fluid can enhance the mass transfer capacity of gas-liquid and enhance the absorption and desorption of carbon dioxide. On the basis of the original experiment, the mixed nanofluid can further expand the experimental effect and control the content of carbon dioxide in the ship's exhaust gas. As a new experimental direction, mixed nanofluid treatment of ship exhaust gas treatment has laid a research foundation for ship energy conservation and emission reduction, and provided a reference scheme for subsequent ship energy conservation and emission reduction experiments.

Carbon dioxide looping on biochar obtained from sewage sludge pyrolyis-gasification

Maria Elena Lozano Fernandez and Norbert Miskolczi

University of Pannonia, Faculty of Engineering, Research Centre of Biochemical, Environmental and Chemical Engineering, MOL Department of Hydrocarbon & Coal Processing, H-8200, Veszprém, Egyetem u. 10, Hungary; lozano.elena@mk.uni-pannon.hu (M.E.L.F.); mnorbert@almos.uni-pannon.hu (N.M)

The further utilization of significant amounts of sewage sludge poses several challenges. The most commonly used ways are not sustainable in the aspect of circular economy. Pyrolysis and gasification of sewage sludge is one of the options for long-term sustainable solutions. Thermal processes produce valuable gas products, liquid products that also contain hydrocarbons, and solid residues (biochar). In connection with the products, the main directions of energy utilization are being researched, however, due to their surface properties and composition, it is worth to investigate other, more value-added applications. This may include the use of biochar in the capture, storage and transport of carbon dioxide. Carbon Capture and Utilization (CCU) or Carbon Capture and Storage (CCS) processes are widely investigated methods for reducing the amount of carbon dioxide released into the atmosphere. Different methods are known for implementing CCS and CCU methods, of which looping methods are widely studied.

This work is dedicated to the investigation of the applicability of biochar obtained from the pyrolysis and gasification of sewage sludge samples under different parameters in carbon dioxide capture. Biochar produced under different parameters had different compositions, morphological and surface characteristics. Carbon dioxide uptake capacity was investigated by TG-FTIR instrument. The results showed that in addition to the bio-char composition, its morphology also had a significant effect on its carbon dioxide capture capacity. In addition to physical processes, chemical processes have also taken place. The Boudouard reaction also had to be expected, especially at higher temperatures.

Keywords: sewage sludge, biochar, looping, pyrolysis, gasification, carbon dioxide

Direct air capture of CO_2 by KOH activated bamboo biochar

Chen Zhang[1], Shuzhuang Sun[1], Su He[1], Chunfei Wu*

[1]School of Chemistry and Chemical Engineering, Queens University Belfast, Belfast, UK BT7 1NN

*E-mail: c.wu@qub.ac.uk

Direct air capture of CO_2 is considered one of the most promising carbon capture methods, and it is expected that direct carbon capture can directly reduce ambient CO_2 concentration to mitigate the greenhouse effect. Biochar is an attractive adsorbent for CO_2 removal because it is environmentally friendly and cost-effective.

In this work, KOH activated bamboo biochar was used as an adsorbent to perform direct air capture using a fixed-bed reactor, and one of the activated biochar shows the highest CO_2 capacity of 51.740 μmol g^{-1}. The effect of relative humidity on the CO_2 adsorption by biochar was investigated and exhibited promising stability under 2.7% relative humidity. However, the biochar activity for CO_2 capture is reduced to 63.88% under 67.1% humidity after 50 cycles.

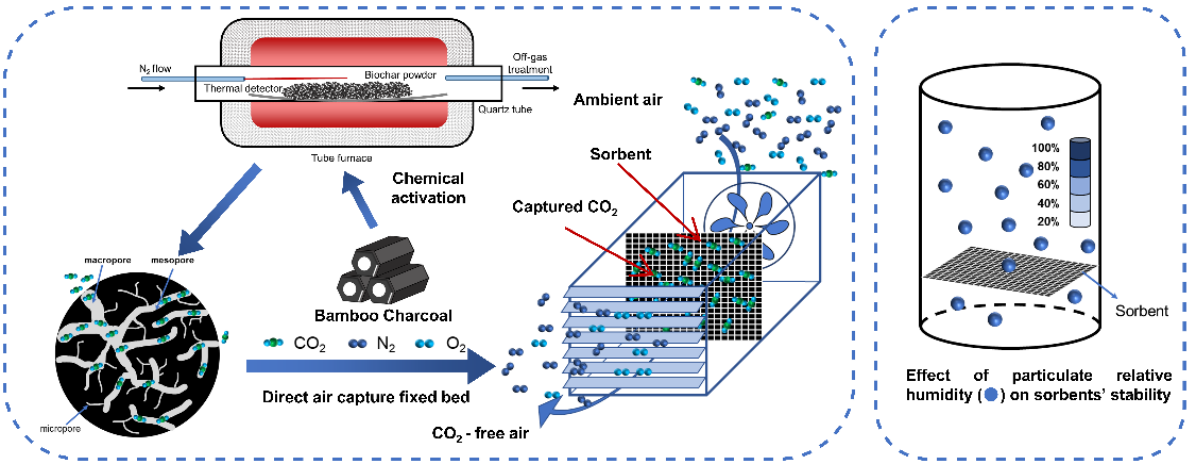

Figure 1: Diagram of bamboo charcoal application in carbon capture.

Ni promoted Fe-CaO dual functional materials for integrated CO_2 capture and reverse water-gas shift reaction

Shuzhuang Sun, Su He, Chunfei Wu*

School of Chemistry and Chemical Engineering, Queen's University Belfast, Belfast, BT7 1NN, UK

*corresponding author: C.Wu@qub.ac.uk

The massive amount of CO_2 emissions caused by the excessive use of fossil energy has a profound impact on the climate, environment and human lives. Carbon neutrality is considered to be one of the most important global targets in the first half of the 21st century. Integrated CO_2 capture and utilization (ICCU) is a promising solution to in-situ reduce carbon emissions and convert CO_2 into valuable products. The integrated process saves equipment and operating costs by omitting the CO_2 enrichment storage and transportation process. Furthermore, the gradually released CO_2 can react with the reducing agent to significantly enhance the CO_2 conversion over ICCU[1].

In addition to causing the greenhouse effect, CO_2 is also an energy storage material. Reverse water-gas shift combined with F-T synthesis is an excellent solution for hydrogen storage and carbon neutrality. Ni and Fe-based materials have been widely applied in reverse water-gas shift reaction[2], however, not been thoroughly investigated in ICCU[3]. Considering the possible industrial application, the ICCU evaluation indicators are still unclear. This report illustrates the advantages and disadvantages of Ni and Fe-based materials under ICCU conditions and the solutions to some critical problems.

Results and Discussion

Ni and Fe possess different ICCU-RWGS performance in terms of CO_2 conversion, CO yield and selectivity. Fe-based catalysts can exhibit better ICCU performance at lower temperatures (< 650 °C). For example, the CO_2 conversion, CO yield and selectivity of Fe_{10}-CaO and Ni_{10}-CaO at 600 °C are 87.3% and 77.8%, 10.9 mmol/g and 2.1 mmol/g, 100% and 93.4%, respectively. Compared with sol-gel CaO without active metals, all materials show enhanced CO_2 conversion. However, the Ni addition affected the morphology of CaO and further decreased the CO_2 adsorption and CO yield performance at a lower temperature. As shown in Figure 1, Ni and Fe-CaO also showed various ICCU cycle performance. The Ni_{10}-CaO possesses improved ICCU performance in cycles, which might be caused by the continuous seepage of metallic nickel from the inside of Ni_{10}-CaO in H_2 atmosphere. In contrast, Fe_{10}-CaO exhibits a significantly higher CO yield and a comparable CO_2 conversion. Furthermore, the Ni_1Fe_9-CaO possesses optimal cycle performance in terms of CO yield and selectivity.

Fe showed better ICCU performance compared to Ni-based material in terms of CO yield and selectivity, however, it generated undesirable in CO_2 adsorption process. Here, we tried three solutions to eliminate the possible CO emission in the adsorption process: (1) N_2 purge by the end of hydrogenation; (2) steam purge after hydrogenation; (3) air purge after hydrogenation.

Figure 2 shows the performance of different solutions on CO production in the adsorption stage. By terminating the hydrogenation process early and using the remaining CO_2 to oxidize Fe, the CO generation in the adsorption stage can be effectively reduced from 1.75 mmol/g to 0.67 mmol/g. However, relying on the release of CO_2 to oxidize Fe is very inefficient and time-consuming. By purging the sample using steam or air for 10 mins can reduce the CO generation in the following adsorption process to 0.13 mmol/g and 0.04 mmol/g, respectively. In short, Fe-based catalysts are a more promising candidate for integrated CO_2 capture and reverse water-gas shift reaction. The drawback of CO generation in the following adsorption process could be effectively hindered by introducing steam or air for a fast purge.

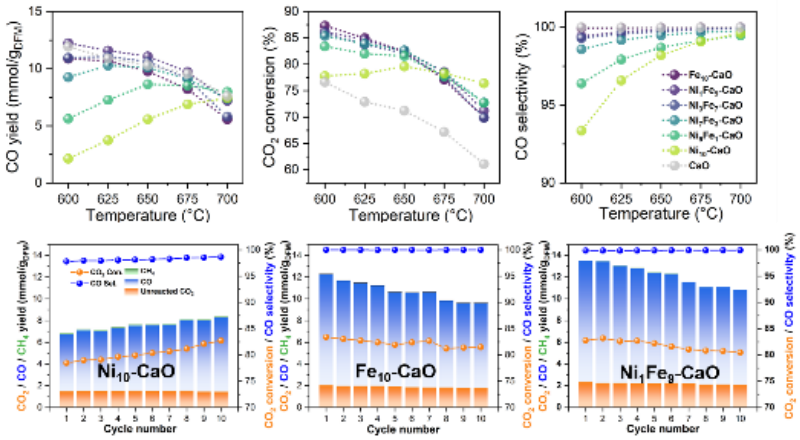

Figure 1.ICCU evaluation performance and cycle test of NixFey-CaO.

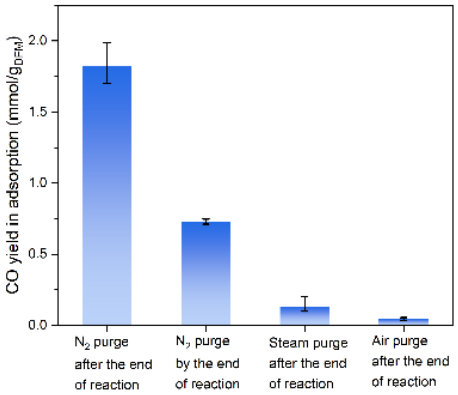

Figure 2. Performance of different solutions on CO production in the adsorption stage

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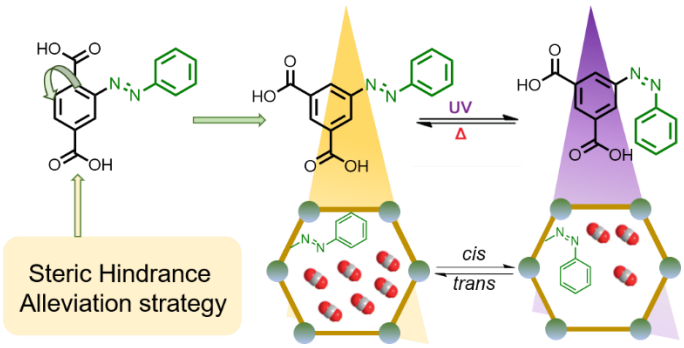
Enhanced Efficiency of Photo Switching Metal-Organic Framework Toward Low Energy Carbon Dioxide Capture

Qi Huang, Chunfei Wu*

School of Chemistry and Chemical Engineering, Queen's University Belfast, Belfast, BT7 1NN, UK

*email: qhuang05@qub.ac.uk, *email:C.Wu@qub.ac.uk*

In the recent decades, many technologies (CCS and CCU) have been attempted to reduce the rising global 2- level. Although some progress had been made, the current state of carbon capture technologies is still relatively expensive and energy intensive. metal organic frameworks (MOFs) because of the high surface area, have been widely reported as adsorbents for gas storage. Photo-switching MOFs are commonly fabricated by incorporating photo-switchable units into MOF materials since they can reversibly change their molecular structure and electronic state through light exposure, such as azobenzene, diarylethene and spiropyran. More importantly, photo switching MOFs prepared via integrating MOF frameworks with photochromic units, can realize the adsorbents regeneration process simply through remote light triggering, which greatly saves the energy cost for MOF adsorbents regeneration. [1]



Herein, we present a strategy to tailor the photo switching efficiency of azobenzene functionalized MOFs via a steric hindrance alleviation approach, which contributed to about 34% enhancement of CO_2 switching efficiency. Thereby, a promising strategy for optimizing the switching efficiency of present photo responsive MOF is explored and verified.[2]

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Development of pilot CO_2 capture membrane system

Zhi Wang

Chemical Engineering Research Center, School of Chemical Engineering and Technology, Tianjin 300072, PR China; Tianjin Key Laboratory of Membrane Science and Desalination Technology, State Key Laboratory of Chemical Engineering, Tianjin Synergetic Innovation Center of Chemical Science and Engineering, Tianjin University, Tianjin 300072, PR China

Carbon capture is one of the most critical technical means to reduce CO_2 emissions. Compared with various carbon capture technologies, membrane separation features operational simplicity, low energy consumption and low ecological footprint, which has attracted wide attention. This report briefly reviews the development of membrane materials, the large-scale preparation of membranes and membrane modules, and then focuses on the simulation and optimization of membrane processes for CO_2 capture, as well as the design and testing of the pilot CO_2 capture membrane systems. Based on the above description, the possible research direction to further develop membrane technology for CO_2 capture is proposed.

Microporous polymer membranes for molecular separations and energy storage

Dr Qilei Song

Department of Chemical Engineering, Imperial College London, UK.

To achieve net zero emissions by 2050, we need to accelerate the development of low-carbon technologies, such as carbon dioxide separation from flue gas, air separation, H_2 purification, and electrochemical devices for energy conversion and storage. Membranes play important roles in these low carbon technologies. Highly permeable and highly selective membranes are desired for these separation and electrochemical processes.

Microporous polymer membranes, such as polymers of intrinsic microporosity (PIMs), present high gas permeability, however, their selectivity is relatively poor, and physical ageing in thin films is limiting their real applications. Therefore, tailoring the distribution, size, and architecture of channels and free volume elements is critical to substantial enhancement of selectivity. I will present our work in membrane manufacturing and post-synthetic transformation, such as thermal and chemical crosslinking. Molecular sieve membranes derived from PIMs polymer show ground-breaking separation performance in terms of gas permeability and selectivity. In additional to separation membranes, we also developed ion-selective membranes by incorporating ion-conductive groups into the polymers. The versatile chemistry of polymer membranes can be tailored on the molecular level to precisely tune the pore size and ion-conducting functionality to match the batteries with different redox chemistries. The new PIM membranes significantly boost battery energy efficiency and peak power density and enable stable operations of RFBs. Our membrane design strategy may inspire the development of a new generation of membranes for a wide range of separation and electrochemical processes.

Water-energy-carbon nexus: A life cycle assessment of post-combustion carbon capture technology from power plant level

Junyao Wang1*, Xuelan Zeng2, Yongzhen Wang3, Shuai Deng4

1 School of Materials and Energy, Guangdong University of Technology, Guangzhou 510006, China
2 Institute of Environmental and Ecological Engineering, Guangdong University of Technology, Guangzhou 510006, China
3 School of Mechanical Engineering, Beijing Institute of Technology, Beijing 100081, China
4 Key Laboratory of Efficient Utilization of Low and Medium Grade Energy (Tianjin University), Ministry of Education, Tianjin 300350, China
*e-mail: wangjunyao_hkust@126.com

Carbon capture and storage (CCS) technology is widely regarded as an important strategy to limit CO2 emissions from point sources, especially for coal-fired power plants. However, current CO2 capture technologies are energy-intensive and require substantial cooling capacities. The extensive deployment of CCS technology increases the energy and water stress in power sectors. This study considers a plant level nexus approach to assess the relationship between water, energy consumption, and CO2 emissions of four types of available post-combustion carbon capture power plants from life cycle perspective.

A technology-based bottom-up approach coupled with the LCA method was employed to develop an analytical framework for the water-energy-carbon nexus. The Integrated Environmental Control Model is a computer-modeling program to calculate the performance of fossil-fueled power plants. This study used IECM to model the energy balance and water consumption for PCC power plants. Next, based on their operational performance, the life cycle assessment method was utilized to access the water, energy, and carbon emissions for various PCC power plants. On the basis of a 650 MWe supercritical power plants (PC) using a wet cooling tower, three feasible PCC technologies, including four scenarios that can be retrofitted to coal-fired power plants were considered in this study: (1) Absorption-based PCC power plant with 30wt % monoethanolamine (MEA) solvent (PC-MEA); (2) Absorption-based PCC power plant with 14.4wt% ammonia solvent (PC-Ammonia); (3) Solid sorbent temperature swing adsorption-based PCC power plant (PC-TSA); and (4) PCC power plant with membrane separation (PC-membrane).

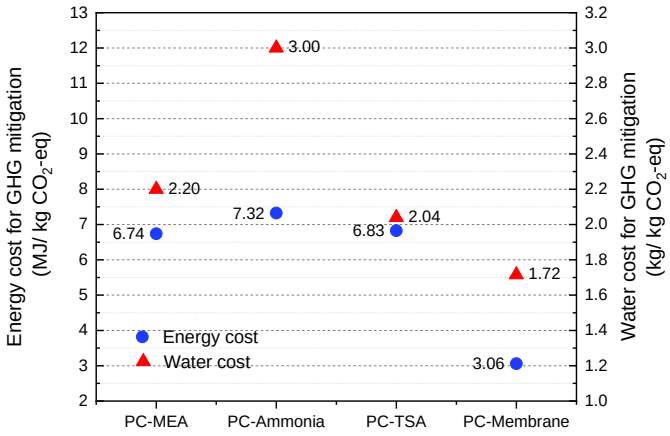

Fig.1 Life cycle water and energy intensity for GHG mitigation

Fig. 1 shows the trade-offs of GHG reductions of PCC power plants. It is found that the integration of CCS translates into an increase in life cycle primary energy demand (PED) by 21~46% and water resources depletion by 59-95% compared with the reference power plant with wet cooling tower system, where the membrane-based system exhibits the best performance. However, the life cycle GHG reduction rate reduced to 65%-70% at 90% capture rate. The life cycle energy and water cost of GHG mitigation were quantified as 3.06-7.32 kJ/kg CO2-eq and 1.72-3.00 kg/ CO2-eq, respectively, demonstrating the presence of sharp trade-offs between GHG reductions and energy demand as well as water consumptions for carbon capture technologies.

Ultra-selective membranes obtained by pre-oxidation of intrinsic microporous polymers for natural gas sweetening

Yatao Weng,[a,b] jianxin Li, *[a,b] Xiaohua Ma*[a,b]

[a] State Key Laboratory of Separation Membranes and Membrane Processes, National Center for International Joint Research on Membrane Science and Technology, Tiangong University, Tianjin, 300387, PR China

[b] School of Materials Science and Engineering, Tiangong University, Tianjin, 300387, PR China

Natural gas is considered as one of the most important green energy alternative to relieve the carbon emission and maintain the energy production. However, till now, almost half of the natural gas generated from the wellhead contains certain amount of CO_2, which must be removed to meet the pipeline standard and achieve the CO_2 capture simultaneously [1].

Membrane technology is considered as one of the most promising techniques to separate CO_2/CH_4 at very low energy consumption whereas maintaining small footprint and investment. However, one biggest challenges lies in this field is the suitable membrane with high permeability, selectivity and reliability. Herein, we made a series of pre-oxidized bromated PIM-1 membrane for CO_2/CH_4 separation testing (**Fig. 1**). Upon changing the treatment temperatures ranging from 300 to 365 °C at the O_2 percentage of 200 ppm, a series of high performance membranes can be obtained. In which, the PBA-350-5 demonstrated a CO_2 permeability of 619 Barrer and CO_2/CH_4 selectivity of 124, which is far beyond the latest 2019 trade-off line. This is contributed by the synergistic effect of bromine and very small O_2 oxidation. When CO_2/CH_4 (50/50) mixed-gas was applied, even at the feeding pressure of 550 psi, the CO_2 permeability in mixed-gas can still reach as much as 306 Barrer combined with CO_2/CH_4 selectivity of 106, which is by far larger than polymer membranes ever reported and showing great perspective in the future natural gas sweetening applications.

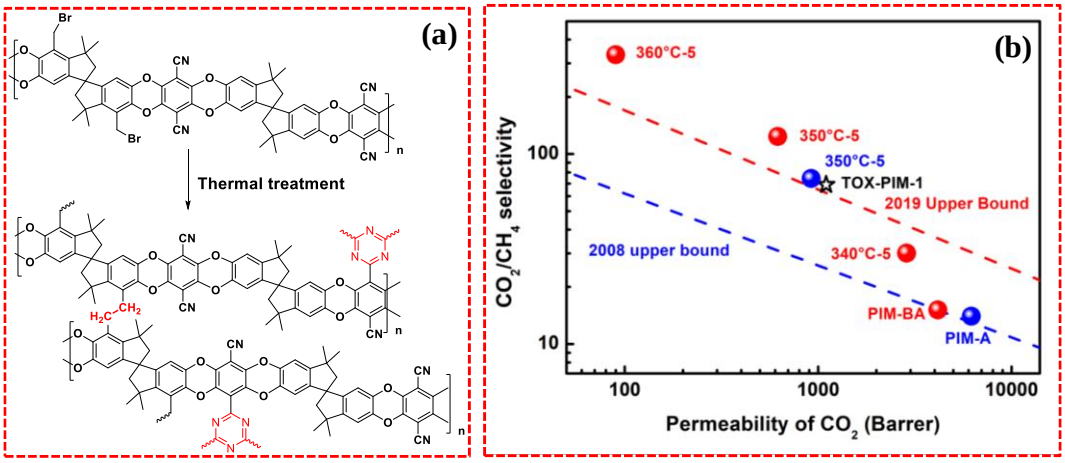

Fig. 1 (a) Structure of the brominated alternative PIM-BA and its proposed cross-linked structure. (b) The CO_2/CH_4 separation performance of PIM-BA thermal treated at different temperatures against their trade-off curves.

Reference

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Cost effective Waste-derived Adsorbents for Post-combustion Carbon Capture

Mikhail Gorbounov, Ben Petrovic, Salman Masoudi Soltani*

Department of Chemical Engineering, Brunel University London, Uxbridge UB8 3PH, United Kingdom
*Corresponding author **E:** Salman.MasoudiSoltani@brunel.ac.uk **T:** +44(0) 1895 265884

Bioenergy with Carbon Capture and Storage (BECCS) has been regarded as one of the most prominent tools to tackle climate change. However, solid residues generated upon combustion of *biomass* pose a separate set of economic and environmental challenges that have to be addressed. Valorisation of this waste stream into low-cost yet effective adsorbents for post-combustion carbon capture is a promising pathway for *in-situ* decarbonisation of the UK biomass combustion energy sector. Therefore, in this work industrial-grade biomass combustion ash generated at a UK power plant has been used as the precursor material for the synthesis of efficient yet low-cost adsorbents for carbon capture. The synthesis method has been optimised *via* design of experiments (DoE) to identify the optimum operating conditions.

Machine Learning in CCUS and Blue Hydrogen Production: Pros and Cons

William George Davies and Salman Masoudi Soltani*

Department of Chemical Engineering, Brunel University London, Uxbridge UB8 3PH, United Kingdom
*Corresponding author **E**: Salman.MasoudiSoltani@brunel.ac.uk **T**: +44(0) 1895 265884

Within the UK, since declaring a climate emergency in 2019 public policy within the context of climate change has shifted to ensuring we reach net zero in comparison to 1990. The government has set a net zero strategy last year. Part of this strategy to ensure we reach net zero is development of carbon capture utilisation and storage (CCUS) technologies, a transition from oil and gas to renewable resources and an increase of hydrogen production.

CCUS has been recognised as a key tool in our decarbonisation efforts to mitigate the effects of climate change. Hydrogen has been identified as a fuel for the future, however; currently hydrogen production is done through the reforming of fossil fuels and produces CO_2 as a by-product. Incorporation of carbon capture technologies with hydrogen production (i.e. blue hydrogen) is key to minimise the CO_2 released into the atmosphere. Both a time and cost-effective way of developing theses technologies is machine learning (ML), using ML to develop these new technologies and expand knowledge within these research areas.

This presentation aims to provide an overview of how machine learning has been utilised so far within these research areas and recommends a future direction for incorporation of ML into blue hydrogen production and CCUS.

Application of CNTs prepared from waste plastic to phase change materials for battery thermal management

Yuanyuan Wang

Queen's university Belfast

Email: ywang135@qub.ac.uk

Carbon nanotube (CNT), possessing excellent thermal properties, is widely utilized as fillers to enhance the thermal performance of phase change materials (PCM) for battery thermal management. CNTs have been demonstrated as promising high-value products from thermal chemical conversion of waste plastics and securing new applications is an important prerequisite for large-scale production of CNTs from waste-plastic recycling. In this study, CNT, produced from waste plastic through chemical vapor deposition (pCNT), was applied as nanofillers in PCM42, affording pCNT-PCM composites. Compared with pure PCM, the addition of 5.0 wt.% pCNT rendered the peak melting temperature increase by 1.3 ℃ (43.7 ℃), latent heat retain 90.7% (197.8 $J.g^{-1}$), and thermal conductivity increase by 104% (0.51 $W.m^{-1}.K^{-1}$). The results of morphological analysis and leakage testing confirmed that pCNT has similar PCM encapsulation performance and shape stability to those of commercial CNT. The formation of uniform pCNT cluster networks allowed for a large CNT loading into the PCM on the premise of free phase change, responsible for the high thermal conductivity inside the homogeneous phase. Thus, the resulting capillary forces retained a high latent heat capacity and suitable melting temperature and prohibited PCM leakage from the matrix to the outside during re-melting as the pCNT loading ratio increased. Therefore, the as-prepared pCNT-PCM composite is a promising candidate for battery thermal management systems.