YONSEI-CBE International Workshop Series:
Separation Technology 2021 (Virtual)

January 12, 2021,
9 AM (Korea Standard Time)

ZOOM Link:
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- **Prof. Kumar Varoon Agrawal**, École Polytechnique Fédérale de Lausanne
  Atomic-thick filters for molecular separation
- **Prof. Zhiping Xu**, Tsinghua University
  Deciphering the nature of ion-graphene interaction
- **Prof. Hae-Kwon Jeong**, Texas A&M University
  MOF-enabled membranes: Innovative approaches toward energy-efficient gas separations
- **Dr. Praveen Thallapally**, Pacific Northwest National Laboratory
  MOF materials and membranes for Xe/Kr removal from nuclear reprocessing plants
- **Prof. Chris Wilmer**, University of Pittsburgh
  Using large scale computational screening to find MOFs for carbon capture applications
- **Prof. Jin Shang**, City University of Hong Kong
  Adsorption-based gas separation and storage for environmental and energy applications

Organized by Prof. Jong Hak Kim, Prof. Youn-Sang Bae, Prof. Dae Woo Kim
Sponsored by BK21 Four, Department of Chemical and Biomolecular Engineering, YONSEI University

Program

January 12, 2021 (Tuesday)

Opening time: **9 AM** (Korea Standard Time)
1 AM (Central European Time)
8 AM (China Standard Time)
7 PM (Eastern Standard Time)

09:00-10:35	**Presider (Prof. Dae Woo Kim, Yonsei University)**
09:00-09:05	Opening Remark (Prof. Jong Hak Kim, Yonsei University)
09:05-09:35	Prof. Kumar Varoon Agrawal
09:35-10:05	Prof. Zhiping Xu
10:05-10:35	Prof. Hae-Kwon Jeong
10:35-10:45	**Coffee Break**
10:45-12:20	**Presider (Prof. Youn-Sang Bae, Yonsei University)**
10:45-11:15	Dr. Praveen Thallapally
11:15-11:45	Prof. Chris Wilmer
11:45-12:15	Prof. Jin Shang
12:15-12:20	Closing Remark (Prof. Jong Hak Kim, Yonsei University)

Atom-Thick Filters for Molecular Separation

Kumar Varoon Agrawal

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Since its isolation from graphite in 2004, graphene has been a part of many exciting developments in the field of basic sciences and engineering. One application that our group is keen on developing is the use of atom-thick graphene film for separating molecules based on their relative size. Achieving such membranes will allow realization of large molecular fluxes, and will significantly cut down the cost of separations in a number of areas including carbon capture, hydrogen generation, paraffin/olefin separation, etc. In this talk, I will discuss the developments in our laboratory on the synthesis of nanoporous graphene-based membranes that allows differentiating gas molecules based on their size. I will discuss the versatility of such approach towards a number of critical separations as well as progress in the scale-up of graphene membranes.

Kumar Varoon Agrawal is an Assistant Professor at the Institute of Chemical Sciences and Engineering (ISIC) at École Polytechnique Fédérale de Lausanne (EPFL) where he heads the laboratory of advanced separations (LAS). He received his Ph.D. in Chemical Engineering from the University of Minnesota working with Prof. Michael Tsapatsis and Prof. Lorraine Francis, where he developed the two-dimensional zeolite nanosheets. In his postdoctoral research with Prof. Michael Strano at the Massachusetts Institute of Technology, he studied the effect of nanoconfinement on the phase transition of fluids. He started his research group at EPFL in 2016 focusing on developing synthetic routes for the two-dimensional nanoporous membranes with a precise control of nanopore size and functionality. He is recipient of North American Membrane Society Young Membrane Scientist Award, European Research Council Starting Grant, Swiss National Science Foundation Assistant Professor Energy Grant among others.

Deciphering the Nature of Ion-Graphene Interaction

Zhiping Xu

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Ion-specific interactions with materials are important for the design of ion-based separation, energy storage and information applications. The problem was studied here with a focus on alkali-earth-metal and transition-metal ions in the context of carbon nanofluidics that have gained attention recently in ion separation applications for their outstanding efficiency.

Density functional theory calculations show that for the alkali-earth-metal ions, the nature of interaction is ionic, with charge transfer to and from graphene determined by the change in work function. In contrast, covalent bonding is identified for transition-metal ions adsorbed on graphene, showing hybridization near the Dirac point. The ion-graphene interaction is significantly stronger than van der Waals interactions and shows much higher contrast among the ions. We find that, surprisingly, these features are robust even with the presence of water solvation, where alkali-earth-metal ion-graphene interaction remains ionic with modified charge transfer, while covalent interaction with transition-metal ions turns into ionic.

These understandings imply that the ion-wall interaction can be notably tuned by the external electric field, as verified by our calculations, and opens an avenue for the development of nanofluidics where the channel width is comparable with the range of ion-wall interaction. The need for experimental measurements of specific ion-graphene interactions and potential approaches will also be covered in the discussion.

Dr. Zhiping Xu is a Professor of Engineering Mechanics at Tsinghua University. He received his B.S. (2002) and Ph.D. (2007) from Tsinghua University and worked at Rice University (2007-2008), MIT (2008-2010) as a postdoctoral researcher before returning to Tsinghua. His research interests include microstructures of matter and their evolution, transport processes and fluid-structure coupling at small scales.

MOF-Enabled Membranes: Innovative Approaches Toward Energy-efficient Gas Separations

Hae-Kwon Jeong

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Molecular sieving metal-organic frameworks (MOFs) offer unique opportunities as membrane materials not only for polycrystalline membranes but also for mixed-matrix membranes (MMMs). Zeolitic-imidazolate frameworks (ZIFs), a sub-class of metal-organic frameworks (MOFs), are of particular interest in gas separations primarily due to their ultra-micropores (pores smaller than 5 Å) and their unusual thermal/chemical stabilities. Despite their potentials, neither polycrystalline MOF membranes nor MOF-containing MMMs have been commercialized due to both fundamental materials and processing challenges.

In this talk, I would like to discuss completely new approaches to address both materials and processing challenges mentioned above. In the first part, I'll talk about the current status of polycrystalline MOF membranes and discuss some of our recent work on increasing productivity of membranes. In the second part, I'll introduce a new approach, PMMOF, to *in-situ* form MOF-containing MMMs, both flat sheets and hollow fibers. I will then briefly discuss the first MMM module containing several MMM hollow fibers.

Jeong earned his Ph.D. in chemical engineering at the University of Minnesota, where his thesis advisor was Michael Tsapatsis. He currently serves as Professor of Chemical Engineering and Materials Science and Engineering at Texas A&M. His research focuses on chemical purification and separation.

Metal Organic Framework Materials and Membranes for Xe/Kr Removal from Nuclear Reprocessing Plants

Praveen Thallapally

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Separation of volatile radionuclides (noble gases) from the off-gas streams of a used nuclear fuel reprocessing facility has been a topic of significant research. The current technology uses energy intensive cryogenic distillation, which is expensive. Another downside of this approach is the accumulation of ozone due to radiolysis of oxygen. Therefore, alternate technologies, and associated materials and membranes, are needed for separation of noble gases over other gases including CO_2, N_2, O_2 and Ar. Pacific Northwest National Laboratory is exploring porous materials including new class of materials called metal organic frameworks (MOFs) for noble gas separation at near room temperature. Our laboratory results demonstrate the small pore MOFs outperform traditional adsorbent materials such as Zeolites at room and low temperature with high adsorption capacity and selectivity. The high selectivity towards noble gases over other gases at low concentration indicates the perfect match between the pore size and the kinetic diameter of the gas species.

Praveen K. Thallapally is Sr. Research Scientist at Pacific Northwest National Laboratory, Richland, WA. His research is focused on the development of multifunctional hierarchical materials, membranes and thin films focused on porous *metal organic frameworks (MOFs), covalent organic frameworks (COFs), and supramolecular hosts (Cucurbituril's, Pillar[n]arene's, calix[n]arene, etc)* for adsorption, separation, extraction, sensing, and catalysis. My research on gas adsorption, separation, adsorption cooling and sensing using materials were published in more than >50 DOE technical reports, >5 US patents and ~150 international peer-reviewed journals, as well as >6 reviews and >5 book chapters with over >10,000 citations and H-index of 61 (Google Scholar).

Designing Electronic Noses with MOFs & Molecular Simulations

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Metal-organic frameworks (MOFs) are promising for chemical separations, catalysis, and gas storage. By changing the building blocks used in their self-assembly, their pore structures can be tuned to target specific applications, and in two decades over 70,000 different MOFs have been reported in the literature. However, quickly finding the best MOFs for any particular gas separation application remains a challenge, as experimental synthesis and characterization can be expensive and time consuming. In contrast, computational simulations of MOF performance can be much quicker and thus can be used to rapidly screen many thousands of candidate materials inexpensively. In this talk, I will discuss a range of simulation methods and results used to identify promising MOFs for different gas separation applications, with a focus on carbon capture. We use classical molecular simulations in combination with continuum models to make predictions about the effectiveness of both adsorbent columns and also mixed-matrix membranes for various carbon capture scenarios.

Besides identifying MOFs with promising gas adsorption characteristics, our lab has recently specialized in also considering thermal properties. Through molecular simulations, we have investigated the thermal conductivity of MOFs both as a function of their pore structure and also as function of gas loading. An important observation of ours is that thermal conductivity of MOFs generally decreases in the presence of adsorbed gases. This observation indicates there are future challenges for MOFs to overcome as gas adsorbents: not only are they typically insulating materials to begin with, but their insulating nature is exacerbated by the presence of gases. In this talk we present our collected evidence on this important phenomenon and outline potential strategies to control and mitigate unwanted thermal effects in gas adsorption scenarios.

Chris was born in Canada to Polish parents who immigrated to Canada shortly before Poland went under martial law in 1981. Spurred by nanotechnology-driven visions of the future penned by writers Erik Drexler and Ray Kurzweil, Chris acquired a B.A.Sc. degree from the University of Toronto's Engineering Science—Nanoengineering program. Coming to the United States to pursue a Ph.D. in Chemical Engineering at Northwestern under the mentorship of Prof. Randall Q. Snurr, he took an interest in the American way of developing new technologies—through entrepreneurship. While still a student, he co-founded, NuMat Technologies, which develops commercial gas storage solutions using MOFs (and has a gas fill plant in Sihwa, South Korea, via its partner, Versum Materials). For co-founding NuMat, Chris was named to the Forbes Top 30-Under-30 list in Energy Innovation. At the University of Pittsburgh, he directs the Hypothetical Materials Lab, whose research focuses on advanced uses of porous crystals, such as for carbon capture, artificial noses, and storing oxygen. His lab recently spun-out Aeronics, which manufactures inexpensive oxygen storage containers for people (and pets!) with decreased lung function. In his ample spare time (that is a joke) he is the managing editor of *Ledger*, the world's first scholarly journal focused on blockchain research, the technology that powers Bitcoin (that is not a joke). He is also a co-author of *"Bitcoin for the Befuddled,"* which has now been translated in Korean!

Adsorption-Based Gas Separation and Storage for Environmental and Energy Applications

Jin Shang

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The gas industry is a 500-billion-dollar input to nearly every sector of the global economy. Separation of gases into their pure components is an important unit operation in chemical industry, accounting for more than 60% of the total cost in many processes. Typical examples are natural gas processing, oil refinery, and environmental remediation. Gas storage in a high-density and safe manner is also crucially important for various applications, including fuel gases for automobiles, natural gas for long-distance transportation, therapeutic medical gases for clinical applications, instrument gases for industry usage, and electronic gases delivery in the semiconductor fabrication processes. Adsorption technology using porous materials can offer highly efficient routes for gas separation and storage applications. In this talk, I will present our recent progress in CO_2 capture, natural gas separation, and NO_2 removal, as well as briefly touch on adsorption-based gas storage.

Dr. Jin Shang is an assistant professor leading GasTech Laboratory (Gas Adsorption, Separation, Storage, and Catalysis) in the School of Energy and Environment at City University of Hong Kong (QS world university ranking 48). He did his PhD in Chemical Engineering at the University of Melbourne and postdoc work at the University of Melbourne and Georgia Institute of Technology. Dr. Shang specializes in molecular adsorption, separation, and storage using porous materials such as zeolites and metal-organic frameworks. His research is focused on understanding the fundamental physical chemistry of the molecular adsorption process via combined experimental and computational methods, in order to rationally develop high-performance adsorbents. The target applications include carbon capture and utilization, methane purification from nature gas/biogas/landfill gas, nitrogen oxides removal and abatement, volatile organic compounds removal, energy gas storage, etc. Dr. Shang has published over 80 papers (h-index 23, citations 1504, as of December 2020) in journals such as Nature Communications, Journal of the American Chemical Society, Angewandte Chemie, etc.