Catalysis Club of Philadelphia

Webinar: 3:30pm EST, Thursday, April 22nd, 2021

Webinar link shared after registration

Speaker : Prof. Sofia Calero

Materials Simulation and Modelling, Eindhoven University of Technology, The Netherlands

Adsorptive Process Designs for Gas Separation using Porous Crystals

Graduate Student Speaker: Julian M. Paige

Department of Chemical and Biomolecular Engineering, University of Pennsylvania

Investigating the Catalytic Requirements of Perovskite Fuel Electrodes Using Ultra-Low Metal Loadings

Meeting Schedule:
3:30 PM: Opening Remarks
3:35 PM: Student Speaker
3:50 PM: Main Speaker

Meeting Fees:
Free to CCP Members

Meeting Etiquette:
Please remember to mute your microphone and arrive early to solve any technical issues.

Webinar Registration:
Please register online by **Wednesday, *April 21st*** using this **LINK** or notify Arrangements Chair Jian Chang (CJ).

A webinar meeting invite will be provided on April 22nd to all those who register.

Membership:
Dues for the 2020-21 season will be $25 ($5 for the local chapter and $20 for the national club). Dues for students, post-docs and retirees will be $10 ($5 for local club and $5 for national club). Use this **LINK** for membership registration.

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Adsorptive Process Designs for Gas Separation using Porous Crystals

Prof. Sofia Calero

Materials Simulation and Modelling, Eindhoven University of Technology, The Netherlands

Abstract:

Gas separation is essential for energy production. In the petroleum industry, isomerization processes generate a mixture of isomers of alkanes that require separation and recycling. There are other possibilities of obtaining refined fuels from raw material different from petroleum that also require gas separation. For example, the Fischer Tropsch Gas To Liquid (FT GTL) process provides liquid hydrocarbons from coal, biomass or natural gas. The process can be optimized by recycling compounds of the flue gas mixture. Related to energy and carbon capture and storage, the separation of hydrogen from carbon dioxide or the effective separation of carbon dioxide, carbon monoxide and oxygen are also essential. Ordered crystalline porous materials, such as zeolites, metal organic frameworks (MOFs) or zeolitic imidazolate framework (ZIFs) offer the potential for selective adsorption exploiting differences in molecular configurations. Zeolites are readily available, very stable and cheap. MOFs and ZIFs are less stable than zeolites, but they exhibit almost unlimited structural possibilities because of the wide variety of combinations of metal atoms, organic linker molecules and the building blocks used in self-assembly during synthesis.

We design conceptual separation processes consisting of several adsorptive steps using a combination of experiments and simulations. Molecular simulation is currently fast and accurate enough to allow rapid evaluation of structures for storage and/or separation devices. For effective separation, one needs to find materials with high adsorption selectivity and with the adequate capacity for use in traditionally used fixed-bed devices. Hence, crystalline structures need to be examined for their ability to conduct gas separation based on adsorption equilibrium, selectivity, diffusion, permselectivity, structural features and kinetics. In most cases the efficiency mostly depends on the optimal combination of selectivity and effective pore volume, and this can be obtained from our simulations and experiments. Using this approach, we designed for example, a double-layered ZIF membranes fabricated inside polyimide P84 hollow fibers for the separation of hydrogen/carbon dioxide mixture (Figure 1). Our hypothesis is that a carbon dioxide adsorption reduction on the surface of the ZIF-9 would enhance the molecular sieving effect of this ZIF layer and therefore the selectivity in the hydrogen/carbon dioxide mixture separation of the entire membrane [1]. Similarly, we found zeolites and MOFs that could be effective materials for the separation of hydrocarbons (e.g. alkanes from alkenes and structural and chiral isomers), and we targeted some zeolites that combined in the correct order could optimize the syngas process, purify natural gas or enhance the capture of carbon dioxide and the recovery of carbon monoxide from gas mixtures [2-4].

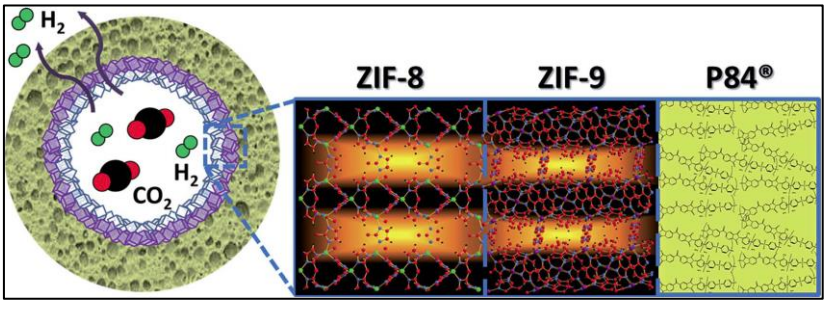

Figure 1. Scheme of the double-layered ZIF-8/ZIF-9 membrane inside a polymeric (P84) hollow fiber for H_2/CO_2 separation

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Speaker's Biography:

Sofía Calero studied Physical Chemistry at University Complutense of Madrid, where she received her MSc degree in 1995. In 2000, she obtained her PhD, cum laude and extraordinary prize, at the same university. From 2001 to 2003 she was a postdoctoral researcher as a Marie Curie Fellow in the Chemical Engineering Department of the University of Amsterdam, the Netherlands. In 2004 she moved to the University Pablo de Olavide, Seville, Spain as Ramon y Cajal Fellow (2004), Profesor Contratado Doctor (2006), Profesor Titular de Universidad (2009) and Catedrático de Universidad (2017). In 2020 she was appointed full Professor and chair Materials Simulation & Modelling at the department of Applied Physics, at Eindhoven University of Technology (the Netherlands). Calero received several grants and awards, including the Marie Curie Excellence Award (2005), ERC Consolidator Grant (2012-2016), Salvador de Madariaga Grant (2016), Dutch VPP-KNAW grant (2017), Spanish Royal Society of Chemistry awards for Young Researchers (2005) and for Scientific Excellence (2018) and Irene Curie Grant (2020). Her research involves the application of molecular simulation to industrially relevant systems and the development of force fields, algorithms and simulation methods to reverse-engineer properties of porous materials.

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Investigating the Catalytic Requirements of Perovskite Fuel Electrodes Using Ultra-Low Metal Loadings

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Abstract:

Solid Oxide Fuel Cells (SOFC) with $La_{0.3}Sr_{0.7}TiO_3$ (LST)–yttria-stabilized ZrO_2 (YSZ) anodes were prepared by impregnation of LST into porous YSZ scaffolds and then modified by Atomic Layer Deposition (ALD) of Ni, Pt, Pd, Fe, Co. and CeO_2. Weight loadings as low as 0.01% of Pt, Ni, and Pd were sufficient to decrease anode impedances by orders of magnitude for operation in humidified H_2 at 973 K. The effects of CeO_2, Co, and Fe were less but still significant. Sintering at higher temperatures was important. Possible ways of stabilizing the metal particles and implications for developing ceramic anodes are discussed

Speaker Biography:

Julian is a 4th year PhD student working in the groups of Raymond Gorte & John Vohs at the University of Pennsylvania. Julian is originally from Odenton, Maryland, and received his B.S. in Chemical Engineering from the University of Maryland Baltimore County (UMBC). His work has focused on using Atomic Layer Deposition to study methods of modifying the catalytic properties of SOFC electrodes as well as heterogenous catalysts.