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The Catalysis Club of Philadelphia

Thursday, January 19th, 2023

Brandywine Plaza Hotel
630 Naamans Road, Claymont, DE 19703

**Enantioselective Catalysts Based on Metal-Organic
Framework-Supported Nucleotides**

Speaker: Prof. Michael Tsapatsis

Johns Hopkins University

**Understanding Polymer-Porous Solid Interactions for
Polymer Upcycling**

Student Speaker: Tian Ren

University of Pennsylvania

Meeting Schedule:

Social Hour 5:30 PM
Dinner 6:30 PM
Meeting 7:30 PM

Meeting Fees:

Members: \$45.00
Non-Members: \$55.00
Stud. & Retired Members: \$35.00

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Meeting and Meal reservations –

Please register online by **Thursday,
January 12th** at

<http://catalysisclubphilly.org/meeting-registration-with-paypal/>

Or contact our Treasurer Steve
Hardwick (sjh.wilm.de@gmail.com) or
Chair Udayshankar Singh
(udayshankar.singh@grace.com)

Membership – Dues for the 2022-23
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 the
local club and \$5 for the national
club).

The Catalysis Club of Philadelphia

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Prof. Michael Tsapatsis

Department of Chemical and Biomolecular Engineering, Johns Hopkins University

Enantioselective Catalysts Based on Metal-Organic Framework-Supported Nucleotides

Danyu Wang, Zhe Li, Tian-Yi Luo, Michael B. Schmithorst, Sunghwan Park, Wenqian Xu, Brandon C. Bukowski, Bradley F. Chmelka, Efrosini Kokkoli and Michael Tsapatsis

Abstract:

We have demonstrated that nucleotides such as ATP could be incorporated into porous materials as a facile method to create a diverse library of heterogeneous asymmetric catalysts. We discovered that well-known metal-organic frameworks can combine several important characteristics to achieve enantioselective heterogeneous nucleotides: (i) irreversible adsorption of the nucleotides through their terminal phosphates; (ii) retention of porosity upon nucleotide incorporation; (iii) inert framework towards (non-enantioselective) catalysis; (iv) affinity for the reactants; and (v) stability in reaction and regeneration conditions, including presence of buffers and extraction solvents.

Although the interaction of nucleotides and metal-organic frameworks has been encountered in the context of efforts to detect nucleotides, irreversible adsorption has not been demonstrated before. We provide crystallographic and spectroscopic evidence on the location of the irreversibly adsorbed nucleotides, which is supported by density functional theory studies.

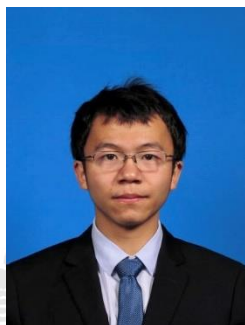
The metal-organic framework supported nucleotides are shown to be stable, reusable, active and enantioselective catalysts using standard probe reactions like Diels Alder and Michael addition.

Speaker Bio:

Michael Tsapatsis is a Bloomberg Distinguished Professor of Chemical and Biomolecular Engineering at Johns Hopkins University (JHU) with a joint appointment in the Applied Physics Laboratory. He received an Engineering Diploma (1988) from The University of Patras, Greece, and MS (1991) and Ph.D. (1994) degrees from the California Institute of Technology (Caltech) working with G.R. Gavalas. He was a post-doctoral fellow with M.E. Davis at Caltech (1993/94). His research group's accomplishments include development of 2-dimensional zeolites, hierarchical meso/microporous zeolite catalysts, and zeolite membranes. His work on zeolites has been recognized by the Donald W. Breck Award (2013) and election to the National Academy of Engineering (2015). Homepage: <https://tsapatsislab.wse.jhu.edu/>



Understanding Polymer-Porous Solid Interactions for Polymer Upcycling



Tian Ren

*Advisor: Prof. Daeyeon Lee & Prof. Raymond J. Gorte
University of Pennsylvania*

Characterization of polymer-solid interactions is critical for understanding the reaction of polymers on catalyst surfaces for polymer upcycling.

In the present study, we measure rates for capillary infiltration of polystyrene (PS) and polyethylene (PE) into disordered packings of silica nanoparticles that had been modified by atomic layer deposition (ALD) with sub-monolayer and monolayer coverages of TiO₂, WO₃, and CaCO₃. Infiltration times depend strongly on the size and surface composition of nanoparticles. The confined infiltration rates measured as a function of surface composition are used to calculate contact angles and interfacial energies for PS and PE via the Lucas-Washburn model. To understand the effect of composition, microcalorimetry measurements with n-hexane and benzene on ALD-modified SBA-15 show a strong correlation between n-hexane adsorption and PE-solid interfacial energies and between benzene and PS-solid interfacial energies.

Except for the surface chemistry, the pore sizes also affect the polymer properties in the porous media, which is called the confinement effect. In our research, the confined viscosities of polymers are determined from the infiltration times via the Lucas-Washburn equation and proportional to 1/pore size in the range from 2 to 20 nm. Another important physics property, confined melting points of PE in the porous media are measured by our cooling and annealing cycles via an ellipsometer. The incremental decrease of melting points increases as the pore size decrease and reach a saturated value of 22°C where the pore size is relatively smaller than the minimum crystalline domain size of PE, the crystalline lamellar size.

The implications of these measurements for understanding reactions on solid surfaces will be discussed in the future.

Speaker Bio

Tian Ren is a 5th year Ph.D. student co-advised by Profs. Daeyeon Lee and Raymond J. Gorte at the University of Pennsylvania. Tian received his bachelor's degree in Chemical Engineering at Tsinghua University in China. His research interests have been the interaction between polymer and solid in nanocomposite and polymer transport in porous media. His current research focuses on the confinement effect and the effect of surface chemistry composition on the polymer-solid interactions in the possible catalytic system for polymer upcycling.