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Promoting Catalytic Science and Technologies

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The Catalysis Club of Philadelphia

Thursday, Nov. 19th, 2026

DoubleTree by Hilton Hotel Wilmington – Wilmington, Delaware

4727 Concord Pike, Wilmington, DE 19803

Machine Learning for Dynamic Catalysis: Atomistic Insights Beyond the Static Surface

Speaker: Prof. Aditya Dilip Lele

Rowan University

Single-step Conversion of Whole Lignocellulosic Biomass into Bio-based Amines

Student Speaker: Dr. Wo Bin Bae

Rowan University

Meeting Agenda:

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

Meeting Registration:

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

Please register online for this In-person meeting by ***Novermber 13th*** at CCP website In-person Meeting Registration — Catalysis Club of Philadelphia.

Meal Selection (Included):

Please make one selection for your dinner (included in registration) when you sign-up for the meeting from the following options:

1. Grilled pork chop with apple & raisin chutney.
2. Boneless beef short rib with peppercorn demi glace.
3. Winter vegetable stew (vegan).

Starter: Butternut squash bisque, toasted pumpkin seeds, dried cranberry
Side: Farro or wild rice and roasted zucchini with yellow squash and peppers

Membership Registration:

Membership dues for CCP 2026-27 meeting 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). Please sign-up membership (Link) for more benefits on meeting registrations and net-working events!

Please contact our Treasurer Gaurav Kumar (gaurav.kumar@dupont.com) or Chair Weijian Diao (weijian.diao@villanova.edu) or Program Chair Jun Hee Jang (jang@rowan.edu) if you need any assistance

catalysisclubphilly.org

General Business

The Catalysis Club of Philadelphia

Thursday, Nov. 19th, 2026



Machine Learning for Dynamic Catalysis: Atomistic Insights Beyond the Static Surface

Prof. Aditya Dilip Lele

Rowan University

Catalysts are rarely static. Surfaces restructure, adsorbates and lattice species migrate, and active sites evolve under reaction conditions, both in conventional thermal processes and in emerging electrified ones driven by rapid heating, plasma, or electrochemical potentials. Density functional theory (DFT) calculations have built much of our mechanistic understanding of catalysis. Extending that understanding to dynamic behavior, however, requires sampling many reactive configurations over long timescales and large length scales. In this talk, I will present our efforts to use machine-learned interatomic potentials (MLIPs) and ML-accelerated atomistic simulations to study catalysis under dynamic and non-equilibrium conditions. MLIPs do more than speed up existing calculations. When combined with transfer learning from foundation models, they make new kinds of calculations practical, from nanosecond-scale reactive dynamics on catalyst surfaces to systematic studies across materials, morphologies, and operating conditions. Drawing on examples from ammonia synthesis and electrocatalysis on transition-metal oxides, I will discuss what these simulations reveal about catalyst behavior under more realistic conditions.

Speaker Bio: Aditya Dilip Lele is an assistant professor in the Department of Mechanical Engineering at Rowan University, with a courtesy appointment in Chemical Engineering. His research group develops ML-accelerated atomistic simulations to understand dynamic and non-equilibrium processes, with applications in thermal, plasma, and electrochemical catalysis, plastic recycling, and the properties of solid-state materials. His work combines density functional theory, reactive molecular dynamics, and machine-learned interatomic potentials, often in close collaboration with experimental groups. He received his M.S. from the Indian Institute of Technology Madras, where he studied biodiesel combustion through chemical kinetic modeling and experiments. He then earned his Ph.D. from Pennsylvania State University, where he used ReaxFF reactive molecular dynamics to study combustion chemistry and developed reactive force

fields for material synthesis. Before joining Rowan, he completed a postdoctoral appointment at Princeton University, where he worked on plasma-assisted catalysis and machine-learned force fields for reactive systems.



Single-step Conversion of Whole Lignocellulosic Biomass into Bio-based Amines

Dr. Wo Bin Bae

Rowan University

Lignocellulosic biomass offers a renewable feedstock for producing nitrogen-containing chemicals and expanding the product application of biorefineries. Conventional routes to biomass-derived amines typically require multiple processing steps, increasing process complexity, cost, and waste generation. This talk presents a one-step strategy that integrates supercritical methanol depolymerization, hydrodeoxygenation, and amination to convert whole lignocellulosic biomass into bio-based amines. Using hybrid poplar as a feedstock, we examine how four nitrogen sources (ammonium hydroxide, ammonium nitrate, urea, and ammonium sulfate) affect biomass conversion and product formation. These compounds serve as nitrogen donors while also affecting biomass depolymerization, leading to differences in product mass balance. The discussion will focus on the role of nitrogen-source selection in coupling biomass depolymerization with amination and its implications for developing streamlined routes to renewable nitrogen-containing chemicals.

Speaker Bio: Wo Bin Bae is a postdoctoral fellowship in Chemical Engineering at Rowan University, under the supervision of Prof. Jun Hee Jang. His research focuses on heterogeneous catalysis and sustainability, with a concentration on catalyst design and understanding reaction mechanisms. He received his B.S in Environmental Engineering and Chemical Engineering from Ulsan National Institute of Science and Technology (UNIST), and his M.S. and Ph.D. in Environmental Engineering from Gwangju Institute of Science and Technology (GIST) in South Korea.