第481回触媒科学研究所コロキウム

Nanocluster Catalysis: Breaking Conventions Through Machine Learning and Artificial Intelligence

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http://www.cat.hokudai.ac.jp/access.html

Abstract

Nanoclusters are pivotal catalysts due to their high surface area and distinct structure–activity relationships. However, conventional approaches often center on larger clusters, overlooking the unique catalytic behaviors of smaller, subnanometer clusters. Recent findings demonstrate that the atomicity of these clusters can dramatically influence their catalytic properties, with even a single atom modification causing significant changes in activity. This talk will explore how machine learning is transforming our understanding of nanocluster catalysis, particularly in examining electronic structures and the impact of external factors. We will also showcase our work on applying machine learning to optimize the catalytic performance of platinum-based nanoclusters in the oxygen reduction reaction (ORR), with a focus on the critical roles of atomicity and relativistic effects.

Biography

Biswarup Pathak is a Professor in the Department of Chemistry at IIT Indore, India, and currently serves as an Associate Editor for ACS Applied Materials & Interfaces. He heads the Computational Materials Designing Research Group at the Institute, where he leads cutting-edge research in computational modelling of nanomaterials, with a strong focus on machine learning and artificial intelligence. Dr. Pathak has published over 300 research articles in internationally renowned journals. His scientific contributions have earned significant recognition, including a feature on the cover of the Journal of Physical Chemistry's Young Scientist Issue. In 2021, he was recognized by the American Chemical Society as one of the most impactful researchers from India. He has also been elected a Fellow of the Royal Society of Chemistry (FRSC), UK.

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