SFU SIMON FRASER UNIVERSITY
ENGAGING THE WORLD

Advanced Catalyst Discovery for Clean Energy Transformation Using Computational Material Design

Samira Siahrostami
Associate Professor, Canada Research Chair
Department of Chemistry, Simon Fraser University

The adoption of sustainable energy sources is crucial for reducing the escalating levels of CO_2 in the atmosphere. To address this issue, renewable energy technologies such as fuel cells and metal-air batteries are poised to play a significant role. In addition, electrolysis cells can help overcome the challenge of producing valuable compounds such as fuels, hydrogen, and ammonia from low-value chemicals like CO_2, H_2O, and N_2. Nevertheless, the lack of efficient catalyst materials poses a significant barrier to the widespread adoption and economic viability of these technologies.

Addressing this challenge requires innovative approaches, and one such avenue is computational catalyst material design and development. By leveraging tools such as density functional theory (DFT), we can develop the atomic scale understanding of surface reactivity, paving the way for the discovery of highly efficient catalyst materials.

In this seminar, I will present our research endeavors on understanding the atomic-scale properties of catalysts using quantum mechanical calculations. By examining their frontiers in various key reactions integral to clean energy processes, we aim to contribute to the advancement of sustainable energy technologies. With various examples, I will show how computational techniques can effectively capture catalytic reactivity trends across diverse chemical space. This approach holds the key to developing novel catalyst materials crucial for propelling the shift towards a greener and more sustainable future.

Short Bio:

Dr. Siahrostami is an Associate Professor of Chemistry and Canada Research Chair at Simon Fraser University in Canada. She previously was an assistant and associate professor at the University of Calgary (2018-2023). Prior to that she worked at Stanford University's Department of Chemical Engineering as a research engineer (2016-2018) and a postdoctoral researcher (2014-2016). From 2011 to 2013, she was also a postdoctoral researcher at the Technical University of Denmark. Her research focuses on using quantum mechanical computational techniques to model reactions at catalyst surfaces. Her goal is to understand the kinetics and thermodynamics of reactions occurring at the surface of catalysts in order to develop more efficent catalysts for fuel cells, electrolyzers, and batteries. She has published over 100 peer-reviewed articles, has an h-index of 48, and has received over 14,700 citations. She has received multiple awards such as 2023 Tom Ziegler Award from the *Canadian Society for Chemistry (CSC)*, 2023 WIN Rising Star Award from *Waterloo Institute of Nanotechnology*, and the Environmental, Sustainability, and Energy Division Horizon Prize: John Jeyes Award from the *Royal Society of Chemistry (RSC)* in 2021.