Understanding the Role of Disorder in Materials Used in Solid Oxide Fuel Cells

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Abstract

The critical challenges related to climate change and energy security could be solved if we can find the champion materials to build sustainable and environment-friendly devices. With this aim in mind, my research leverages leading-edge computational techniques and a multidisciplinary approach to understand the behavior of complex electrolytes currently used in solid oxide fuel cells (SOFCs) and optimize them for next-generation fuel cell devices. The electrolytes used in SOFCs are generally polycrystalline with different grain sizes, grain orientations, dopant segregation, and defects distribution. In addition, they are typically characterized by a high density of grain boundaries and interfaces. All these features can substantially affect their ionic conductivity. In this talk, I will discuss our recent findings on the microstructural, ionic, and electronic behavior of grain boundaries and interfaces present in commonly used ceramic electrolytes used in SOFCs. By integrating the classical and quantum simulations, this work prepared realistic models of the working-class materials and provided the long-sought explanation for the experimentally observed phenomenon. Finally, in this talk, I will discuss some of the challenges in identifying the overall impact of all the microstructural defects present in polycrystalline materials and the role that machine learning tools can play in resolving them.

About the speaker

Kulbir Kaur Ghuman is an early-career researcher, recently appointed as Assistant Professor at Institut national de la recherche scientifique, Centre Énergie Matériaux Télécommunications (INRS-EMT) and a Tier-2 Canada Research Chair in 'Computational Materials Design for Energy and Environmental Applications'. Before joining INRS-EMT she worked as a postdoctoral fellow at University of Toronto (2013-2016) and Kyushu University, Japan (2017-2019). Her current laboratory, Insilico Matters Laboratory (IML), is equipped with advanced software and computational infrastructure, dedicated to understanding the theoretical underpinnings of the behaviour of complex materials and chemical reactions. She has established several novel structure-property relationships and mechanisms for optimizing fuel cell materials and designing efficient catalysts imperative for mitigating climate change. Currently, she is also spearheading a recently established consortium 'Computational Energy Materials Design Infrastructure (CEMDI)' at INRS-EMT that aspires to foster innovation in the area of energy materials research via collaboration and advanced computational techniques.