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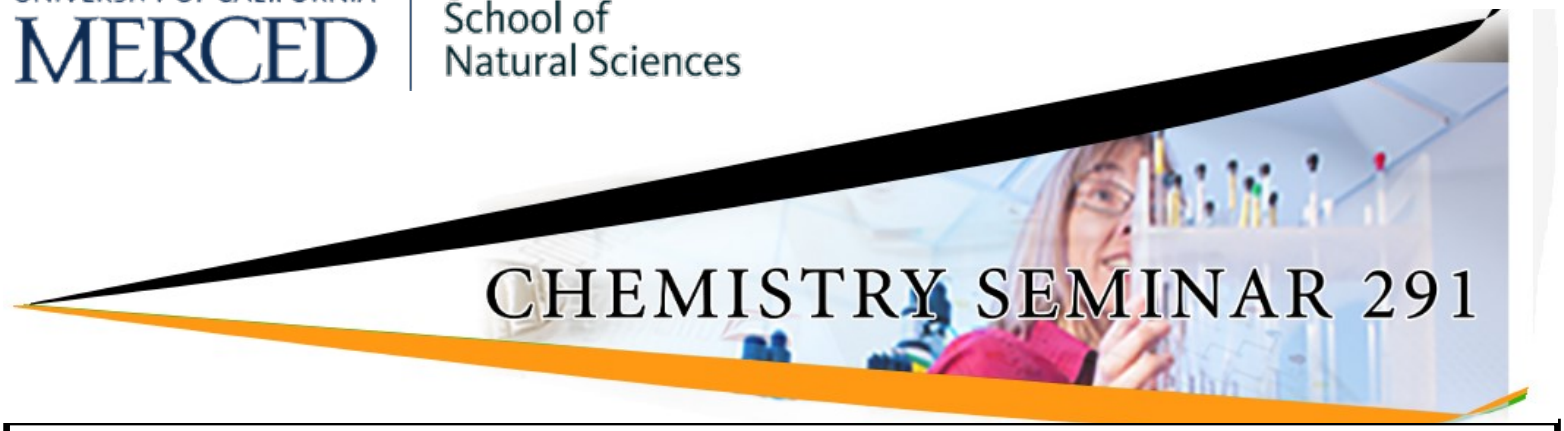


# Understanding the Importance of Active Minorities in Energy Conversion and Storage

Date: **11/22/2019**

Time: **3:00 PM**

Location: **COB1 267**

**David Prendergast**

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## Abstract

Functional materials systems - solar cells, batteries, catalysts - present diverse chemical environments that can be challenging to predict within computational models. Similarly, previously unforeseen agents are difficult to identify within measurements on the same systems. However, developing theoretical models capable of describing such systems with molecular detail and their associated measurable observables is vital to propelling rational advances in materials development. In this presentation, we reveal some surprising details of electrolyte composition that have recently emerged in our molecular dynamics simulations and associated consequences for electrochemical systems. For the most part, we rely on first-principles predictions of spectroscopy to validate our results. We will also explore the importance of such simulations for interpreting an emerging set of complex experiments devoted to the study of active interfaces using X-ray and infrared photons.

## About the Speaker

David Prendergast is the interim Director of the Molecular Foundry, a national user facility for nanoscale science funded by the US Department of Energy at Berkeley Lab. Dr. Prendergast is a computational scientist with a PhD in Physics from University College Cork, Ireland (2002). He worked as a postdoc at Lawrence Livermore National Laboratory with Prof. Giulia Galli (currently at the University of Chicago) and at UC Berkeley with Prof. Steven G. Louie. His current research focuses on developments and applications of first-principles electronic structure theory and molecular dynamics in the context of energy-relevant phenomena in materials and chemistry. He has particular expertise in the simulation and interpretation of synchrotron X-ray spectroscopy measurements as a means of connecting characterization of complex interfacial systems to atomistic or molecular scale structural and dynamical models.