



## PHYSICS COLLOQUIUM:

# Novel Materials for Energy Applications from First Principles

Date: **1/31/2020**

Time: **10:30–11:50 AM**

Location: **COB2 140**

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### Abstract

An active area of research is the search for new materials for solar energy and carbon emission mitigation applications. The ability to synthesize and probe new materials classes with tunable structure and composition – such as 2d crystals, organic semiconductors, halide perovskites, and metal-organic frameworks – has driven the need for new intuition linking atomic- and molecular-scale morphology and phenomena relevant to function, such as photophysics, carrier dynamics, and chemical kinetics. Here, I will present applications of novel first-principles computational methods – drawing on density functional theory and ab initio many-body perturbation theory formalisms – for predicting and understanding the electronic structure, photoactive excited states, and chemical dynamics in these systems. Time permitting, I will cover recent work on the photophysics of 2d semiconductors, singlet fission in acene crystals, the nature of excitons in halide perovskites, and the design of metal-organic frameworks for CO<sub>2</sub> capture. In each case I will share how new theoretical developments, and calculations carried out in close collaboration with experiments, advance our intuition and influence the design and synthesis of new energy materials.

### About the Speaker

Jeffrey B. Neaton is a professor of physics at the University of California, Berkeley, where his research interests include developing and applying theories and novel computational methods to predict, understand and control phase behavior and electronic phenomena in complex materials from first principles. He serves as the Associate Laboratory Director for Energy Sciences at Lawrence Berkeley National Laboratory, overseeing the Chemical Sciences and Materials Sciences Divisions, as well as the lab's two Basic Energy Sciences-sponsored national scientific User Facilities, the Advanced Light Source and the Molecular Foundry. He is also a senior faculty scientist at Berkeley Lab and a member of the Kavli Energy NanoSciences Institute at Berkeley. He is the Associate Director of the Center for Computational Study of Excited-State Phenomena in Energy Materials at Berkeley Lab. He received his PhD degree in physics under Neil Ashcroft from Cornell University, and was a postdoctoral fellow at Rutgers University. After having worked as a postdoc and staff scientist at the Molecular Foundry, he served as Director of the Molecular Foundry from 2013-2019. Neaton is a recipient of a DOE Presidential Early Career Award for Scientists and Engineers award and is a fellow of the American Physical Society. He is the recipient of a NERSC High Impact Scientific Achievement Award in 2017 and was the 2018 Pariser-Parr Distinguished Lecturer in Chemistry at the University of North Carolina.