Quantum Design of Materials for a Sustainable Future

Friday, February 18th, 2022
12:30 PM

Bowen Hall, Room 222

MAE Seminar Series

Emily A. Carter
Princeton University

15 years ago at Princeton I began working on the design of materials for sustainable energy technologies, using quantum-based simulation techniques developed in my group, as well as those of others. 15 years on, I view sustainable electricity generation as largely solved (though storage requires further innovation) and have turned my attention, especially in the past five years or so, to sustainable fuel and chemical production, with a particular emphasis on carbon dioxide utilization and negative emissions technologies. We work to understand and then design electro-, photo-, and thermochemical catalysis enabled by optimal materials and either renewable electricity or sunlight. I will introduce our embedded correlated wavefunction (ECW) theory, which overcomes failures of conventional quantum simulation methods (density functional theory, DFT) so that excited electronic states and charge transfer that are ubiquitous in photo/electro catalysis are properly simulated. We have used this technique to extract mechanistic insight that enables the design and discovery of new materials for solar thermochemical production of syn gas, electrochemical water splitting, (photo)(electro)chemical carbon dioxide reduction, and more.

Emily A. Carter is once again the Gerhard R. Andlinger '52 Professor in Energy and Environment and Professor of Mechanical and Aerospace Engineering at Princeton, while being newly appointed as Senior Strategic Advisor for Sustainability Science at Princeton Plasma Physics Laboratory, as of 2022. She was UCLA's Executive Vice Chancellor and Provost, and a Distinguished Professor of Chemical and Biomolecular Engineering from 2019-2021. Prior to her leadership of UCLA, she had been Princeton's Dean of Engineering and Applied Science (2016-19) and before that, Princeton's Founding Director of the Andlinger Center for Energy and Environment (2010-2016). Dr. Carter develops and applies quantum mechanical simulation techniques to enable discovery and design of molecules and materials for sustainable energy and carbon mitigation technologies. The author of nearly 450 publications and patents, Dr. Carter has delivered over 570 invited and plenary lectures worldwide and has served on advisory boards spanning a wide range of disciplines. She is the recipient of numerous honors, including election to the U.S. National Academy of Sciences, the American Academy of Arts and Sciences, the U.S. National Academy of Inventors, the U.S. National Academy of Engineering, and the European Academy of Sciences.

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