First Principles Solid State Quantum Mechanics Methods for Sustainable Energy: From Fuel Cells to Fusion

A talk by Emily A. Carter
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"Freihaus"- building, 9th floor, "yellow" – Wiedner Hauptstraße 8-10

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To preserve the planet for future generations, we must make major science and engineering breakthroughs in the way we harvest, store, transmit, and use energy. My team contributes to this effort by developing fast yet accurate quantum mechanics simulation methods used to investigate materials and phenomena related to sustainable energy. My current research portfolio includes: evaluating new materials for photovoltaics and photocatalytic electrodes to convert sunlight into electricity and fuels, quantifying biofuel combustion kinetics, optimizing ion and electron transport in solid oxide fuel cells, evaluating mechanical properties of lightweight metal alloys for fuel-efficient vehicles, and investigating liquid lithium for fusion reactor walls. The latter two projects exploit a promising technique - orbital-free density functional theory (OFDFT) - that directly evaluates electron distributions instead of wavefunctions. This method is orders of magnitude faster than standard DFT and as such it can be used to study many thousands of atoms with quantum mechanics. Consequently, OFDFT is able to explicitly study, e.g., plasticity in metals and liquid metal dynamics. Recent advances in both theory and applications will be discussed. Time permitting, we will also present our embedded correlated wavefunction theory that permits a proper treatment of charge transfer, unlike standard DFT. Applications to solar fuels and fuel cell processes will be highlighted.