

O 47: Invited Talk Emily Carter

Time: Wednesday 14:15–15:00

Location: HE 101

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Ab Initio Treatment of Strongly Correlated Electron Materials — ●EMILY CARTER — Department of Mechanical and Aerospace Engineering and Program in Applied and Computational Mathematics, Princeton University, Princeton, NJ 08544 USA

Density functional theory (DFT) has been anointed as the method of choice for a quantum mechanics description of molecules and materials, but it is best used as a qualitative indicator because its quantitative accuracy is still limited by approximate electron exchange and correlation (XC). Moreover, there are cases where DFT fails completely, even in a qualitative sense. Photochemistry, strongly correlated systems,

physisorption, and polymers are all at best poorly described within standard DFT. We will discuss two ab initio techniques we have been developing in order to accurately treat excited states and strongly correlated electrons in condensed matter. In particular, we will discuss our embedded configuration interaction theory, which offers a locally improved description of XC, and an ab initio version of the so-called LDA+U method for strongly correlated materials. We will discuss applications of these techniques to problems where DFT fails (for various reasons that shall be outlined in the talk): the Kondo effect (transition metal impurities in nonmagnetic metallic hosts) and properties of first row transition metal oxides.