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## **DFT+DMFT calculations in oxide superlattices** CHRIS MARIANETTI, Columbia Univ

While density functional theory (DFT) is a useful tool for understanding transition metal oxides and their heterostructures, it can break down qualitatively for certain properties or in specific transition metal oxides. We present a dual variable theory, density functional theory plus dynamical mean-field theory (DFT+DMFT), which remedies many of the shortcomings of DFT. Our full implementation of this method uses a plane wave basis and maximally localized Wannier functions to create the correlated subspace. We will demonstrate the ability to compute not only spectra and low energy properties, but also fully charge self-consistent total energies. We will explain the role of the double-counting correction, and introduce a more optimal approach. The method will be applied to various nickelate superlattices, and we will identify a new class of polar Mott insulators. Additionally, we will address the "thinness" driven metal-insulator transition which is observed in nickelates with very few layers.