Contribution ID: **163** Type: **invited talk**

Strain effects in correlated transition metal oxides from first principles

Thursday, 19 September 2013 09:30 (30 minutes)

Transition metal oxides exhibit a wealth of fascinating and potentially useful properties, such as metal-insulator transitions, multiferroic behavior, or high-temperature superconductivity. The unique electronic structure of these materials generally leads to a very strong coupling between their structural, electronic, and magnetic properties. We are using first principles electronic structure calculations and combinations of such first principles calculations with model-based approaches to explore the unique properties of functional complex oxides. Here, I will address the question of whether epitaxial strain, which is present in most thin film samples as a result of the lattice mismatch between the thin film material and the substrate, is able to induce metal-insulator transitions in the prototypical correlated oxides LaTiO3 and SrVO3. Furthermore, I will demonstrate how Wannier functions can be used to connect the realistic electronic structure calculated from first principles to simplified models, which allow to better understand the interplay between spin, orbital, and lattice degrees of freedom in complex oxides.

Primary author: EDERER, Claude (ETH Zurich)

Presenter: EDERER, Claude (ETH Zurich)

Session Classification: Functional Materials