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Electronic and Magnetic Properties of Transition-Metal Oxide Nanocomposites: A Tight-Binding Modeling at Mesoscale.[1] YUAN-YEN TAI, Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA, JIAN-XIN ZHU, Theoretical Division and Center for Integrated Nanotechnologies, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA — Transition metal oxides (TMOs) exhibit many emergent phenomena ranging from high-temperature superconductivity and giant magnetoresistance to magnetism and ferroelectricity. In addition, when TMOs are interfaced with each other, new functionalities can arise, which are absent in individual components. In this talk, I will present an overview on our recent efforts in theoretical understanding of the electronic and magnetic properties TMO nanocomposites. In particular, I will introduce our recently developed tight-binding modeling of these properties arising from the interplay of competing interactions at the interfaces of planar and pillar nanocomposites. Our theoretical tool package will provide a unique capability to address the emergent phenomena in TMO nanocomposites and their mesoscale response to such effects like strain and microstructures at the interfaces, and ultimately help establish design principles of new multifunctionality with TMOs.

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