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Atomic and Electronic Structures of the Cu2O/TiO2 Heterostructure Interface SHUZHI WANG, BALASUBRAMANIAM KAVAIPATTI, JOEL AGER, Lawrence Berkeley National Laboratory, RAMAMOORTHY RAMESH, University of California, Berkeley, LIN-WANG WANG, Lawrence Berkeley National Laboratory, LAWRENCE BERKELEY NATIONAL LABORATORY COLLABORATION, UNIVERSITY OF CALIFORNIA, BERKELEY COLLABORATION — Earth-abundant metal oxides have great potentials in replacing Si in semiconductor solar cells and meeting the terawatt scale global energy demand. The structural and electronic properties of the heterojunction interface in oxide-based thin film solar cells, which is of great importance to the energy conversion efficiency, however, is not well understood yet. In this talk, we will present our experimental and theoretical work on the atomic and electronic structures of the interface of Cu_2O and anatase TiO_2. Despite the large lattice mismatch of 13%, Cu_2O can be grown epitaxially on $TiO_2(001)$ in the cube-on-cube orientation by pulsed laser deposition. The interface is found to form a regular coincidence lattice of 8 Cu_2O and 9 TiO_2 unit cells in each in-plane direction. The relaxed structure of this coincidence lattice is simulated using density functional theory calculations. The local density of states along the interface is found to shift as much as 0.4 eV, depending on the local alignment of the two lattices. As a result, the valence band and conduction band edge wave functions are well separated.

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