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**The Electronic Structure of Nonpolar Surfaces in Insulating Metal Oxides** DANYLO ZHEREBETSKYY, LIN-WANG WANG, Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA — Understanding the electronic and geometric structures of metal oxide surfaces has a key interest in many technological areas. A randomly chosen crystal surface has a high probability of being polar, unstable and containing in-gap states due to surface dangling bonds. As a result, the surface should be stabilized by passivation or reconstruction. However, do the nonpolar surfaces of ionic crystals of insulating metal oxides need the passivation or reconstruction similar to covalent crystals? We address this question by analyzing the nonpolar surfaces and their electronic structure for the common crystal structures of metal oxides. The study using periodic DFT calculations is performed for following representatives: Cu2O, ZnO, Al2O3, TiO2, V2O5, WO3, CaTiO3, Mg2SiO4. It has been shown that the nonpolar surface can be constructed out of dipole-free, charge-neutral and stoichiometric unit cells for each crystal. We demonstrate that all constructed and relaxed nonpolar surfaces of the metal oxides show a clear band gap. It should be emphasized that the constructed surfaces are neither reconstructed nor passivated. Additionally, we show a correlation between the electronic structure of the relaxed surfaces and Ewald energies calculated for the surface ions.

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