Abstract Submitted
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Antisite defects at oxide interfaces[1] HANGHUI CHEN, ANDREW MILLIS, Columbia Univ — We use ab initio calculations to estimate formation energies of cation (transition metal) antisite defects at oxide interfaces and to understand the basic physical effects that drive or suppress the formation of these defects. We find [1] that antisite defects are favored in systems with substantial charge transfer across the interface, while Jahn-Teller distortions and itinerant ferromagnetism can prevent antisite defects and help stabilize atomically sharp interfaces. Our results enable identification of classes of systems that are more and less susceptible to the formation of antisite defects and motivate a range of experimental studies and further theoretical calculations to further explicate the oxide interface systems. [1] H. Chen and A. J. Millis, arXiv:1509.06643, (2015).

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