Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Ab initio design of low work function complex oxides for thermionic energy conversion STEPHANIE MACK, UC Berkeley, GUO LI, Molecular Foundry, LBNL; Joint Center for Artificial Photosynthesis, JEFFREY NEATON, UC Berkeley; Molecular Foundry, LBNL; Kavli Energy Nanosciences Institute at Berkeley — Understanding and controlling work functions, or band edge energies, is of interest for a variety of applications in optoelectronics and energy conversion. In particular, while recent advances in device design have improved the feasibility of thermionic generators, new low work function materials are needed to enable their widespread use. Perovskite-based oxides (ABO_3) are a diverse class of materials that, depending on the transition metal atoms on the A and B sites, can give rise to myriad emergent and collective phenomena. Here, we use density functional theory calculations to examine how the work function of one such oxide, $SrRuO_3$ (SRO), can be tuned by monolayers of $SrTiO_3$ (STO) and other polar or near-polar oxides. We find that SRO work functions can be tuned by over 1 eV with one layer of STO, although the calculated reduction in work function is an order of magnitude less than would be expected from the bulk polarization. We understand the variation in work function via a detailed analysis of Born effective charges at the surface, which are as small as 10% of their bulk values, and charge rearrangement at the STO surface and SRO/STO interface.

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Date submitted: 06 Nov 2015 Electronic form version 1.4