Abstract Submitted
for the DPP12 Meeting of
The American Physical Society

Work Functions of Sc_2O_3 surfaces containing Ba/BaO for thermionic electron emitters using Density Functional Theory RYAN JACOBS, JOHN BOOSKE, DANE MORGAN, University of Wisconsin- Madison — The work functions of (001), (011) and (111) bixbyite Sc_2O_3 surfaces with adsorbed Ba atoms, Ba-O dimers, and rocksalt BaO films have been calculated using Density Functional Theory (DFT) to investigate the role Ba plays in producing the low experimental scandate cathode work functions of ∼1.1-1.4 eV. Our lowest calculated work function was 1.48 eV for a single rocksalt film layer of BaO (011) on Sc_2O_3 (011). Work functions for Ba atom and Ba-O dimer adsorption on Sc_2O_3 (011) and (111) surfaces ranged between 2.1 to 3.7 eV, and depended on the Sc_2O_3 surface termination, coverage density, and adsorption geometry employed. We found the total work function change of a surface with adsorbed species can be decomposed into two parts: the dipole component and Fermi level shift component. The dipole component is described by the Helmholtz equation, and takes into account charge transfer into valence band states and surface charge rearrangement. The Fermi level shift is a result of either mobile charge transfer into conduction band states, or a restructuring of the valence band, which can also modify the work function.

Ryan Jacobs
University of Wisconsin- Madison

Date submitted: 11 Jul 2012 Electronic form version 1.4