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Work Functions of Sc$_2$O$_3$ surfaces containing Ba/BaO for
thermionic electron emitters using Density Functional Theory RYAN JA-
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The work functions of (001), (011) and (111) bixbyite Sc$_2$O$_3$ 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 ex-
perimental 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$_2$O$_3$
(011). Work functions for Ba atom and Ba-O dimer adsorption on Sc$_2$O$_3$ (011) and
(111) surfaces ranged between 2.1 to 3.7 eV, and depended on the Sc$_2$O$_3$ 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.

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