Work Functions of Alkali and Alkaline Earth Metal Surfaces under Electric Fields based on First-principles Calculations

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Alkali (Li, Na, K, Rb, Cs) and alkaline earth metal (Be, Mg, Ca, Sr, Ba) are widely used in various fields. In the field emission, the adsorption of alkali metals and alkaline earth metals to tungsten (W) will greatly change the work function. In this work, we study the work functions and local work functions of alkali and alkaline earth metal (100) (110) (111) surfaces under different electric fields using the first-principles or *ab initio* calculations. The convergence of density-functional-theory (DFT) calculations in the local-density approximation (LDA) and generalized-gradient approximation (GGA) with a plane-wave basis set the projector-augmented wave method as implemented in the Vienna ab-initio simulation package (VASP) has been carefully and systematically tested. For a comparison, the work functions have been calculated with five different pseudo potentials. By applying an electric field on the alkali and alkaline earth metals, we can calculate the effective work function, local work function and investigate the dependence of the effective work function and the local work function on the field strength.

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