Local work functions of clean tungsten surfaces under electric fields based on *ab initio* calculations

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Tungsten, the common choice for vacuum tube filaments, can survive under high temperatures and provide thermionic emission of electrons. However, the emission is largely limited due to its relatively high work function (approximately 4.5 eV). First principles or *ab initio* calculations are used to study the local work functions of tungsten (W) clean (100), (110), and (111) surfaces under external electric fields. The authors carefully and systematically tested the convergence of density-functional-theory (DFT) calculations in the local-density approximation (LDA) or 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). Several pseudopotentials have been tested for comparion. With the tungsten model under electric fields applied on both sides, we can investigate the dependence of the local work function and effective work function on field strength. In addition to thermionic emission, tungsten has been considered for use as a field emission (FE) electron source.

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