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Calculating work functions with density functional theory: the effect of finite temperature, surface alloying, and oxidation THOMAS R. MATTSSON, DWIGHT R. JENNISON, Sandia National Laboratories, Albuquerque, NM 87185-1186, USA. — The work functions for W, Cu, and Al are calculated using density functional theory (DFT). We go beyond the perfect lattice at zero Kelvin by employing molecular dynamics techniques. Effects of surface alloying and -oxidation are also investigated. The effect of alloying and oxidation is, as expected, found to be significant, while the temperature dependence, although clearly seen, is in comparison weak. In addition, the exchange-correlation density functional AM05 is compared to the results of LDA and PBE. The calculated work functions compare well to available experimental results. This work was supported by the LDRD office and the simulations were performed at the High Performance Computing facilities at Sandia National Laboratories, NM. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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