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What is the work function of a small nanocrystal? LINGYUAN GAO, JAIME SOUTO, ALEX DEMKOV, JAMES CHELIKOWSKY, Univ of Texas, Austin — The work function is defined as the difference between the electrostatic potential energy (-eϕ) of an electron in the vacuum near the metal surface and the metal's Fermi energy. For a single crystal metal, the measured work function typically depends on the orientation of the metal surface. This seems counterintuitive, as the Fermi energy is the same across the metal sample, and the vacuum energy is also expected not to depend on the direction. The problem becomes even more interesting for a metallic nanocrystal, where facets of different orientation meet. We investigate this problem using the real space first-principles method PARSEC and consider aluminum nanocrystals as a test system. The real space nature of the code doesn't require periodic boundary conditions and enables calculations of nanocrystals with realistic dimensions. We compare our nanocrystal results for (001), (110) and (111) Al surfaces with those obtained from standard slab calculations and available photoemission and electrical data. We acknowledge supports from SciDAC program, Department of Energy, Office of Science, Advanced Scientific Computing Research and Basic Energy Sciences. This work is supported through grant DE-SC0008877

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