

Abstract Submitted
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From facets to facets: how does work function vary over a gold nanocluster? LINGYUAN GAO, JAIME SOUTO, JAMES CHELIKOWSKY, ALEX DEMKOV, Univ of Texas, Austin — Owing to their potential applications in catalysis, gold nanoclusters are a focus of intense research. The work function Φ , which can be measured using photoemission spectroscopy is a key parameter used to characterize the catalytic performance of the cluster. Φ is determined by the difference between the electrostatic potential just outside the metal surface and the Fermi energy of the cluster. We use a relativistic version of the real space first-principles code PARSEC to compute the work function of gold nanoclusters with dimensions on the order of a nanometer, which is similar in size to those used in experiment. We illustrate how the work function depends on the surface orientation of the nanocluster facets and compare our results with available experimental data. We acknowledge supports from SciDAC program, Department of Energy, Office of Science, Advanced Scientific Computing Research and Basic Energy Sciences grant DE-SC0008877 for work on algorithms. Two of us (JRC and JS-C) acknowledge support for the work on nanostructures from grant from the U.S. Department of Energy: DE-FG02-06ER46286.

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