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Quantum Monte Carlo Calculations of Pt Nanoclusters and (111) Surface WILLIAM PARKER, ANOUAR BENALI, Argonne National Laboratory, LUKE SHULENBURGER, Sandia National Laboratory, JEONGNIM KIM, Oak Ridge National Laboratory, NICHOLS ROMERO, Argonne National Laboratory, JEFFREY GREELEY, Purdue University — Although density functional theory (DFT) has been successfully used to analyze problems in surface catalysis and electrochemistry at a molecular level, there are several important classes of problems where DFT fails spectacularly, predicting incorrect adsorption energies and binding sites. Better understanding these failures and benchmarking methods for correcting them motivates a quantum Monte Carlo (QMC) investigation of platinum nanoclusters and the platinum (111) surface. To evaluate the transferability of our platinum pseudopotential, we first present the fixed-node diffusion Monte Carlo (DMC) equation of state and cohesive energy for fcc platinum. We then show the binding energies of icosahedral nanoclusters with increasing size and the (111) surface energy to lay the groundwork for investigation of adsorption on these catalytically important phases of platinum.

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