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Potential Energy Functions for Metal Clusters and Nanoparticles[1] NICOLE LEGENSKI, ROBERT C. FORREY, Department of Physics, Penn State University, Berks Campus, HANSONG CHENG, Department of Chemistry, National University of Singapore — Atomic force fields for simulating copper, silver, and gold clusters and nanoparticles are developed. Potential energy functions are obtained for each metallic system using an embedded atom method with parameters that have an explicit dependence on coordination number. Many cluster configurations of varying size and shape are used to constrain the parametrization for each system. Binding energies for these training clusters were computed using density functional theory (DFT) with the Perdew-Wang exchange-correlation functional in the generalized gradients approximation. Extensive testing shows that the many-body potentials are able to reproduce the DFT energies for most of the near-equilibrium and many of the non-equilibrium structures that were included in the training set. Implications for molecular dynamics simulations and extensions to binary metallic systems and also to hydrogen on metallic clusters are discussed.

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