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Ab-Initio Density Functional Calculation of Interatomic Potentials for Large-scale Atomistic Material Simulations. G.L. ZHAO, Department of Physics and High Performance Computing Laboratory, Southern University and A&M College, Baton Rouge, Louisiana 70813, S. YANG, Department of Physics, Southern University and A&M College — We propose a new method to calculate interatomic potentials, utilizing an ab-initio density functional formalism. The calculated interatomic potentials can be used for large scale atomistic material simulations and predictions. We benchmark the method for the case of copper. We utilized the ab-initio interatomic potential to calculate various properties of transition metal copper, including the lattice constant, the bulk modulus, thermal expansion coefficient, monovacancy formation energy, and phonon frequencies. The calculated results agree very well with experimental values. We further calculated the properties of BCC Cu, utilizing the interatomic potential derived from the electronic structure calculations of FCC Cu, to demonstrate the predictive capabilities of the interatomic potential. The predicted properties of BCC Cu agree very well with experimental and ab-initio density functional results. Part of the work was performed during the stay of G. L. Zhao at Princeton University. The authors gratefully acknowledge the financial support of the National Science Foundation (Award No. 0508245).

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