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NRL Tight-Bindind Model for Alkali Metals LEI SHI, George Mason University, DIMITRIOS PAPACONSTANTOPOULOS, Naval Research Laboratory
— We have extended our studies with the NRL tight-binding method to the alkali metal column of the periodic table. The method was applied to Potassium, Rubidium and Cesium. We fit APW calculations of high symmetry structures onto a non-orthogonal tight-binding Hamiltonian. This Hamiltonian accurately reproduces the APW band structures, density of states and total energies as a function of volume. In addition, the tight- binding scheme determines various quantities that were not fitted, such as elastic constants, phonon frequencies and vacancy formation energy in agreement with experimental values. We explore the applicability of this model in performing molecular dynamics simulations. In addition, we will provide comparison with a recent improvement to Harrison's tight- binding theory[1]. [1]Lei Shi and Dimitrios A. Papaconstantopoulos, Phys. Rev. B, 70, 205101(2004).

Lei Shi
George Mason University

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