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First-principles and Tight-binding Calculations in the Pd-H System A. SHABAEV, D.A. PAPACONSTANTOPOULOS, Department of Computational and Data Sciences, George Mason University, Fairfax, VA 22030, USA — Using the linearized augmented plane wave(LAPW) method we have generated a large database of electronic structure results that include fcc, bcc, NaCl, CsCl, Cu3Au, Fluorite crystal structures as well as supercell configurations with various hydrogen occupations for the Pd-H system. The formation energies and energy bands from this database were used to construct a tight-binding model that reproduces well the above LAPW results and, in addition, is transferable to other crystal lattices including random occupation of crystal sites as well as treating vacancies. We calculate the phonon frequencies, elastic constants, the density of states, coefficient of thermal expansion, mean-squared displacement and the energy of vacancies formation in Pd. The objective of this work is to be able to perform electronic structure calculations for systems containing up to a few thousand atoms where first- principles calculations are computationally intractable. This approach is used in both static and dynamic calculations and enables us to vary the amount of hydrogen entering into the Pd matrix.

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