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Structural Phase Transitions & Equation of State of Aluminum from First Principles XIA LU, SATHYA HANAGUD, Georgia Institute of Technology — EOS of Al and the associated structural phase transitions are of special interest in characterizing the mixture of Al with other metal oxides or metals to produce dual functional structural energetic materials. From first principles, we studied the phase transitions of Al at pressures up to 800 GPa and temperatures up to 1000 K. In the past, phase transitions fcc $\diamondsuit$ hcp $\diamondsuit$ bcc were studied at 0K. In this paper, by considering electronic and lattice thermal contributions, we present a phase diagram of Al by investigating the stability of the three phases at pressures and temperatures of interest. Phonon analysis is used for analyzing the phase structural stability. The free energy, due to the cold-curve, electronic and lattice thermal contributions, is used to calculate the EOS with phase transitions. The predicted EOSs are compared with experimental EOSs. Changes of the electronic structures and phonon characteristics with pressure and phase transitions are also discussed. Calculations at ground state are in the framework of DFT, using local density or generalized gradient approximation, and projector augmented wave method. The lattice thermal contributions are obtained by populating the quasiharmonic phonon modes, according to the Boltzmann statistics; the electronic thermal contributions by populating the electron band structures, according to the Fermi-Dirac statistics.

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