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Hard-sphere variational CPMD approach GERALD FAUSSURIER, CHRISTOPHE BLANCARD, CEA, PIER LUIGI SILVESTRELLI, Padova University, CEA COLLABORATION, PADOVA UNIVERSITY COLLABORATION — We present a variational method to determine the total free energy of the electron and ion system using the Gibbs-Bogolyubov inequality and a hard-sphere reference system applied to the quantum molecular dynamics code CPMD. Numerical results and comparisons with quantum molecular dynamics simulations and experiments are presented and discussed for dense and expanded aluminum.

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