

Numerical Simulation

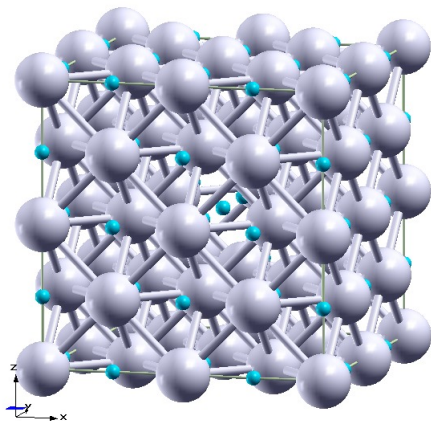
Eunsil Baik

November 20, 2013



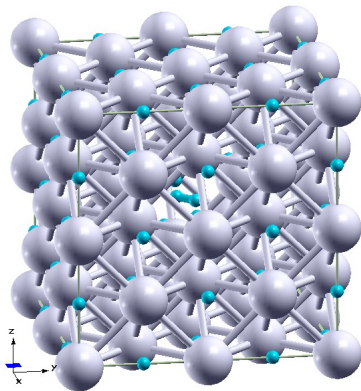
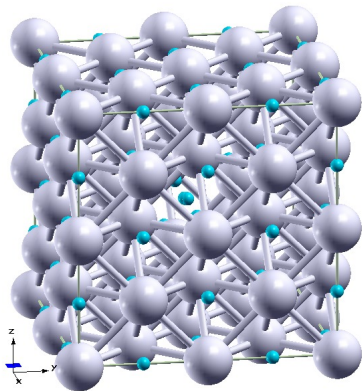
PdH Bulk Vacancy: One H Atom

Total Energy = -24901 eV



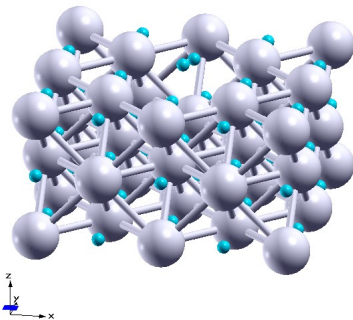
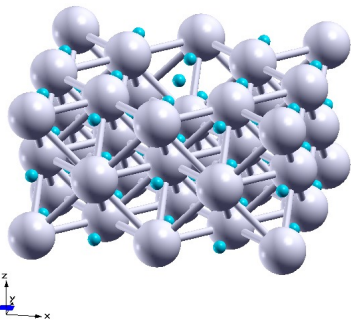
PdH Bulk Vacancy: Two H Atom

Total Energy = -24835 eV to -24918 eV



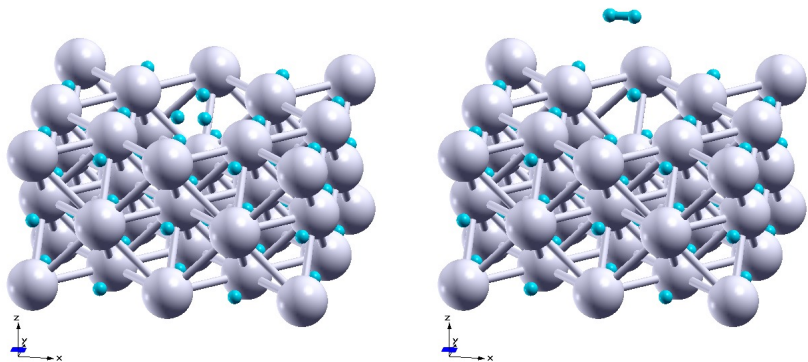
PdH Surface Vacancy: One H Atom

Total Energy = -18475 eV



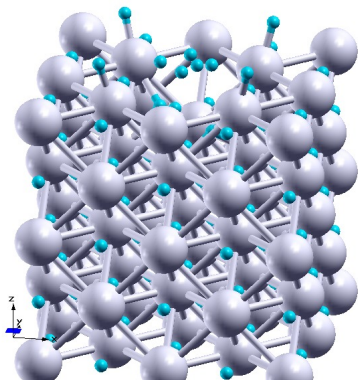
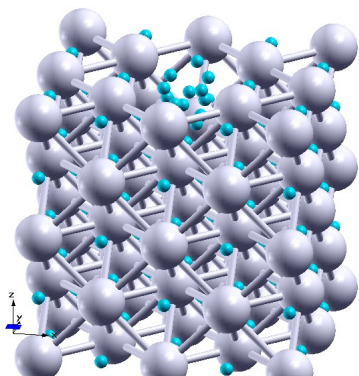
PdH Surface Vacancy: Two H Atoms

Total Energy = -18492 eV to -18493 eV

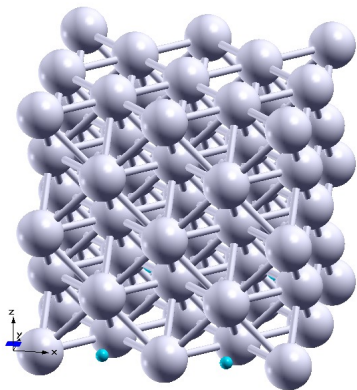


PdH Surface Vacancy: 12 H Atoms

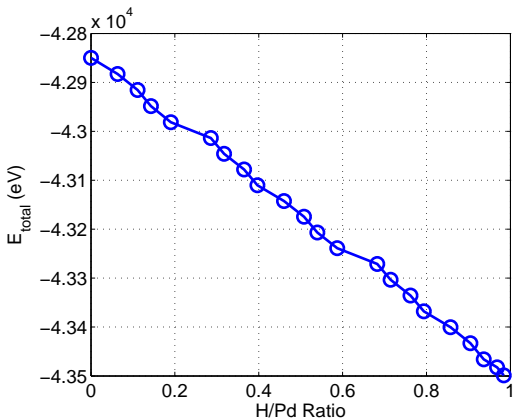
Total Energy = -42583 eV to -42613 eV



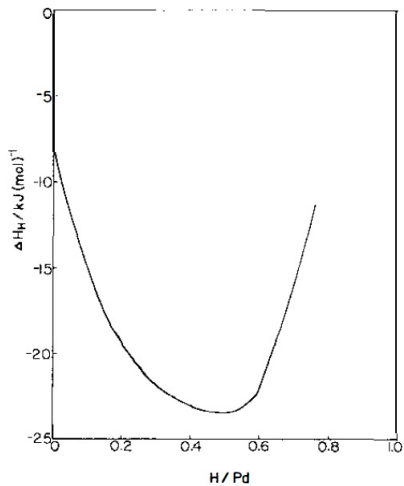
Hydrogen Loading Ratio



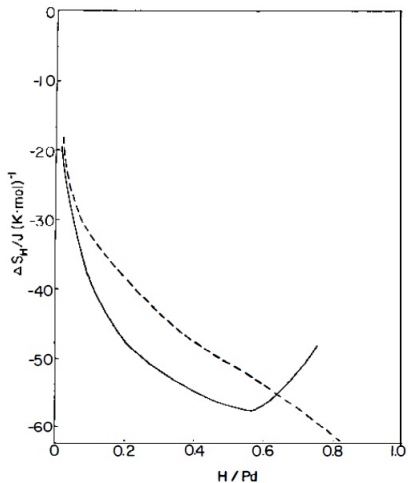
Total Energy vs. Hydrogen Loading Ratio



Enthalpy vs. Hydrogen Loading Ratio



Entropy vs. Hydrogen Loading Ratio



PdH Bulk Vacancy

