

Numerical Simulation

Eunsil Baik

August 14, 2013



Outline

- 1 Computational Method
- 2 Fully Saturated PdH System without Electric Field
 - Geometry Configuration
 - Results
- 3 Fully Saturated PdH System with Electric Field
 - Geometry Configuration
 - Results
- 4 Current and Future Simulations

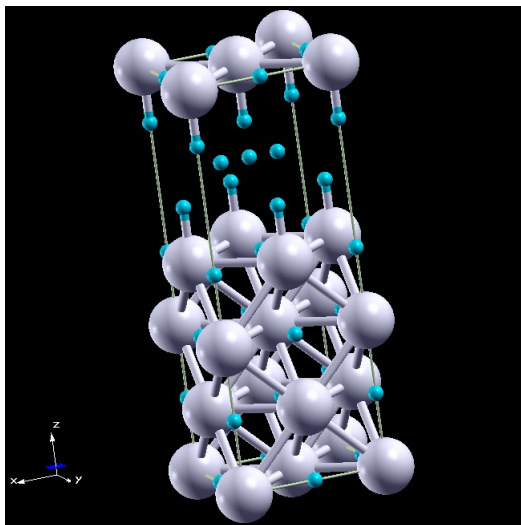
An *ab initio* Study

- Quantum Espresso PWscf (Plane-Wave Self-Consistent Field) code
- Density Functional Theory (DFT)
- Generalized Gradients Approximation (GGA) for Exchange-Correlation Effects
- Ultrasoft Pseudopotential
- Brillouin Zone, K-Points, and Cut-off Energy

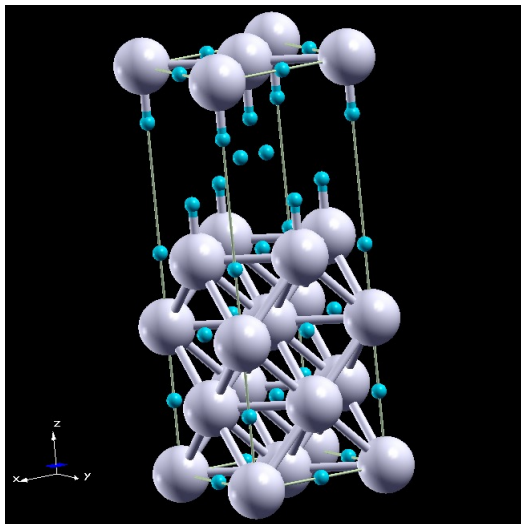
Outline

- 1 Computational Method
- 2 Fully Saturated PdH System without Electric Field
 - Geometry Configuration
 - Results
- 3 Fully Saturated PdH System with Electric Field
 - Geometry Configuration
 - Results
- 4 Current and Future Simulations

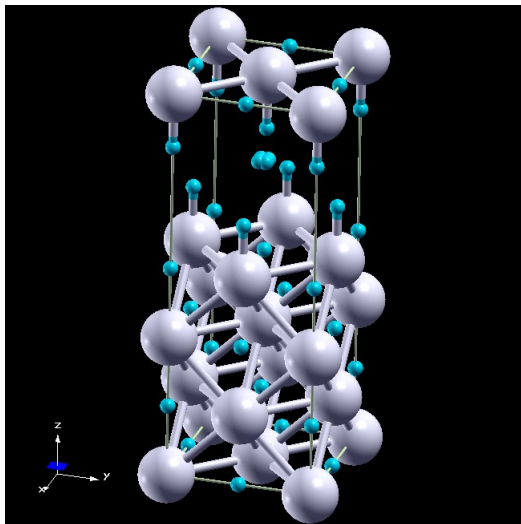
PdH-3H



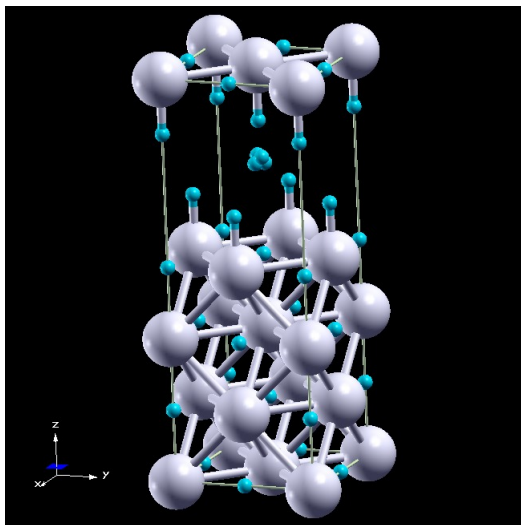
PdH-2H



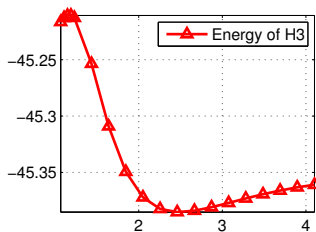
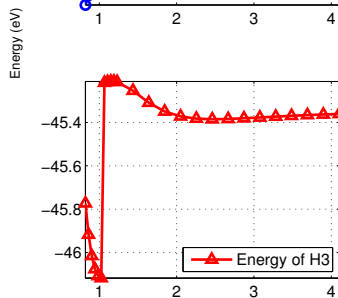
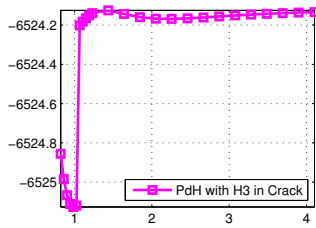
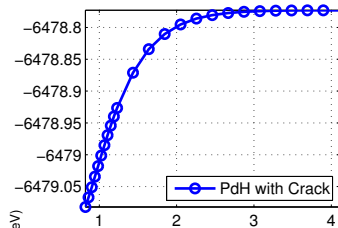
PdH-4H



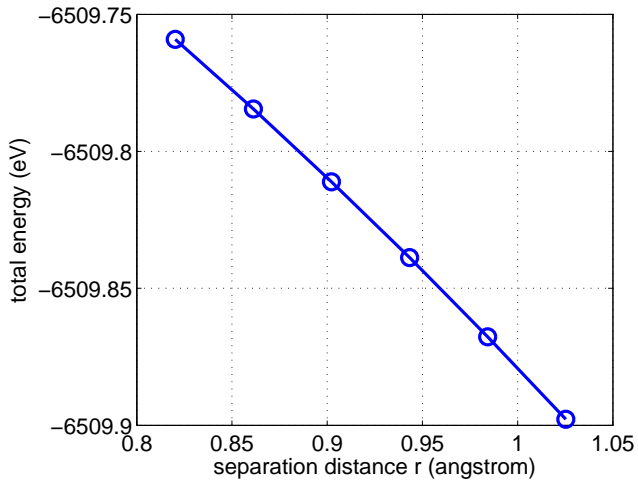
PdH-4H TSC



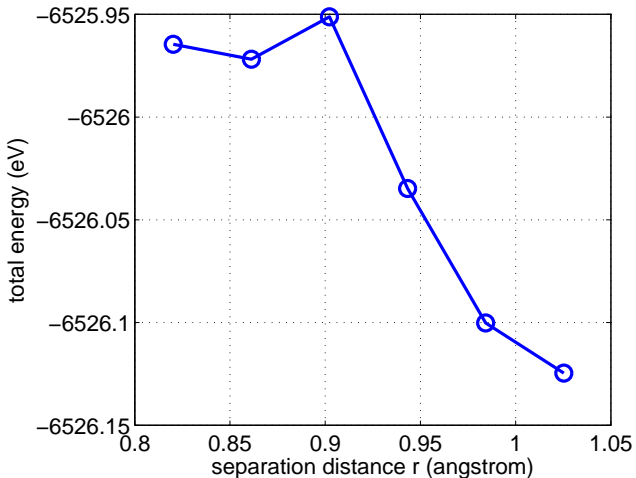
3H Energy Plot

 r (angstrom)

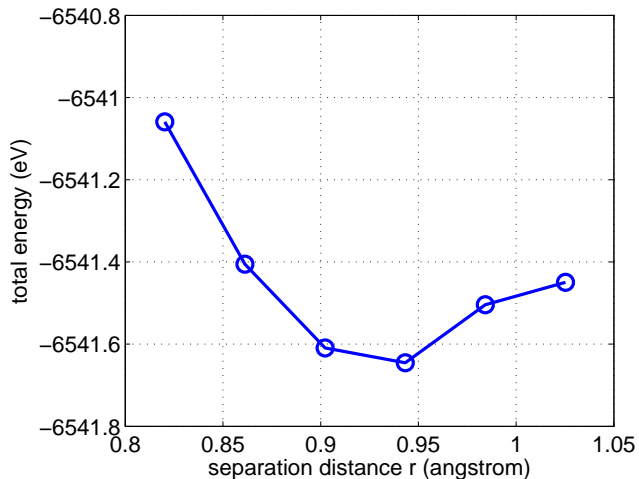
2H Relaxation Energy Plot



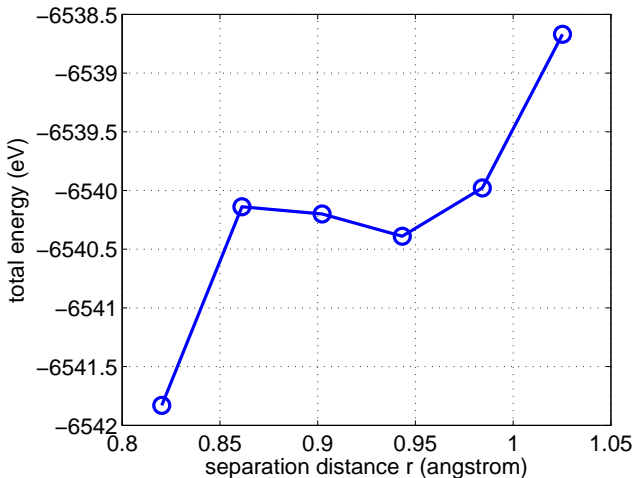
3H Relaxation Energy Plot



4H Relaxation Energy Plot



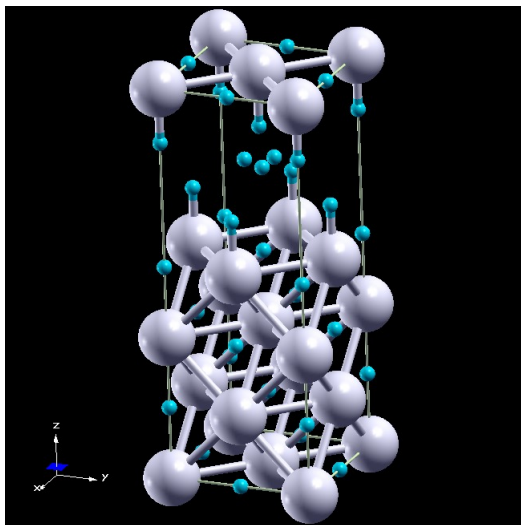
4H-TSC Relaxation Energy Plot



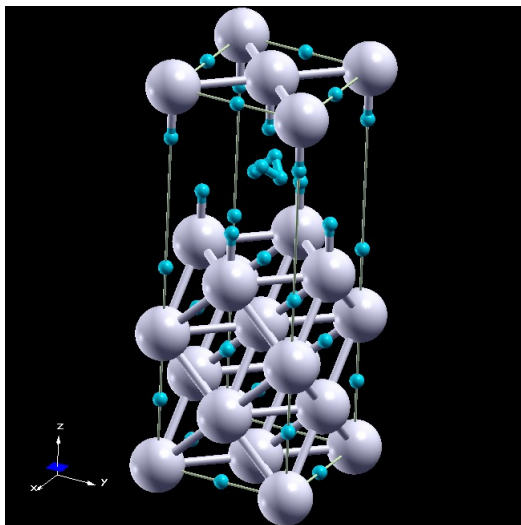
Outline

- 1 Computational Method
- 2 Fully Saturated PdH System without Electric Field
 - Geometry Configuration
 - Results
- 3 Fully Saturated PdH System with Electric Field
 - Geometry Configuration
 - Results
- 4 Current and Future Simulations

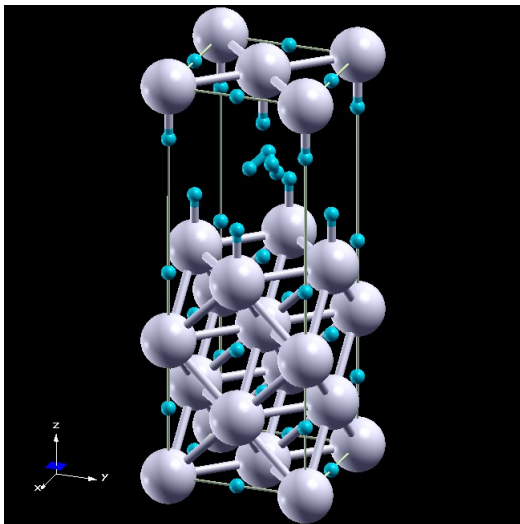
PdH-3H



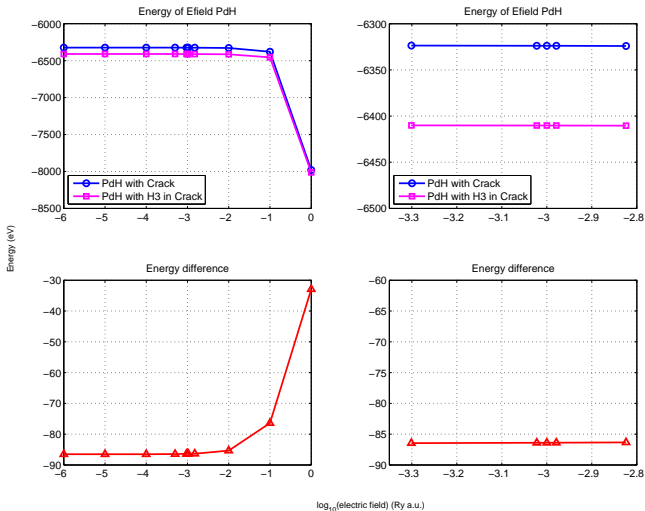
PdH-4H TSC



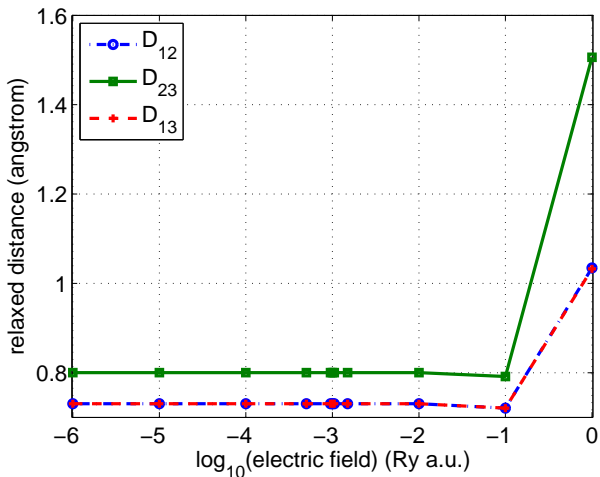
PdH-4H Asymmetry



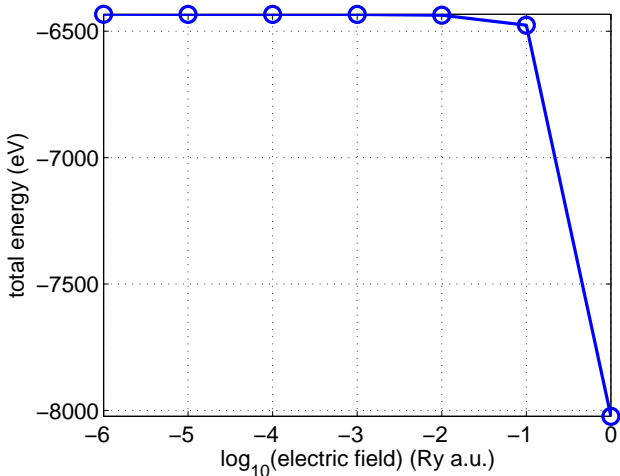
PdH-3H Energy vs. E-field Plot



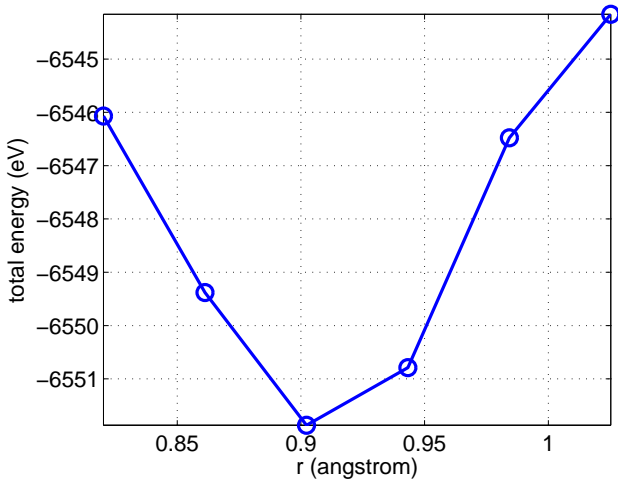
PdH-3H Relaxation Distance Plot



PdH-4H Relaxation Energy Plot



Energy vs. r Plot for E-field is 0.1 (51.4 V/nm)



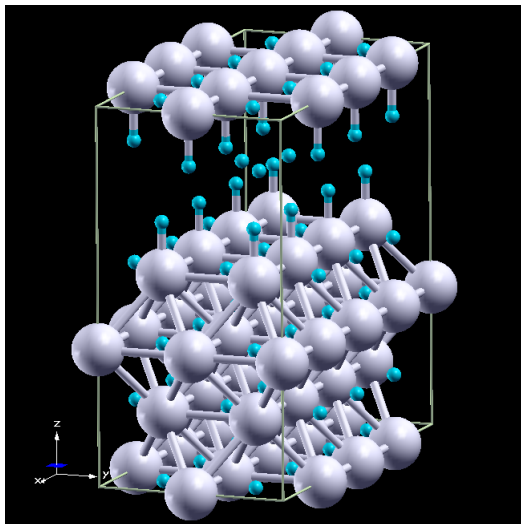
Outline

- 1 Computational Method
- 2 Fully Saturated PdH System without Electric Field
 - Geometry Configuration
 - Results
- 3 Fully Saturated PdH System with Electric Field
 - Geometry Configuration
 - Results
- 4 Current and Future Simulations

Now...

- PdH 100 with z-direction e-field of 0.01 and 0.001
 - 3H model for different r
 - 4H TSC model for different r
 - 4H asymmetric TSC model for different r

Later... PdH10



Later... PdH110

- PdH 110 without electric field
 - 3H model for different r
 - 4H TSC model for different r
 - 4H asymmetric model for different r
- PdH 110 with electric field
 - 3H model for different r
 - 4H TSC model for different r
 - 4H asymmetric model for different r