Eunsil Baik

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Outline

Computational Method

- 2 Fully Saturated PdH System without Electric Field
 - Geometry Configuration
 - Results
- Fully Saturated PdH System with Electric Field
 Geometry Configuration
 - Restuls



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

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Fully Saturated PdH System without Electric Field Geometry Configuration





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Fully Saturated PdH System without Electric Field Geometry Configuration





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Fully Saturated PdH System without Electric Field Geometry Configuration





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Numerical Simulation Fully Saturated PdH System without Electric Field Geometry Configuration

PdH-4H TSC



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Fully Saturated PdH System without Electric Field

Results

3H Energy Plot



r (angstrom)

Fully Saturated PdH System without Electric Field

Results

2H Relaxation Energy Plot



Fully Saturated PdH System without Electric Field

Results

3H Relaxation Energy Plot



Fully Saturated PdH System without Electric Field

Results

4H Relaxation Energy Plot



Fully Saturated PdH System without Electric Field

Results

4H-TSC Relaxation Energy Plot



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- 3 Fully Saturated PdH System with Electric Field

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- Geometry Configuration
- Restuls



Numerical Simulation Fully Saturated PdH System with Electric Field Geometry Configuration





Numerical Simulation Fully Saturated PdH System with Electric Field Geometry Configuration

PdH-4H TSC



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Numerical Simulation Fully Saturated PdH System with Electric Field Geometry Configuration

PdH-4H Asymmetry



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Fully Saturated PdH System with Electric Field

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PdH-3H Energy vs. E-field Plot



log₁₀(electric field) (Ry a.u.)

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Fully Saturated PdH System with Electric Field

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PdH-3H Relaxation Distance Plot



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Fully Saturated PdH System with Electric Field

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PdH-4H Relaxation Energy Plot



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Fully Saturated PdH System with Electric Field

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



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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

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Numerical Simulation Current and Future Simulations

Later... PdH110



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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

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