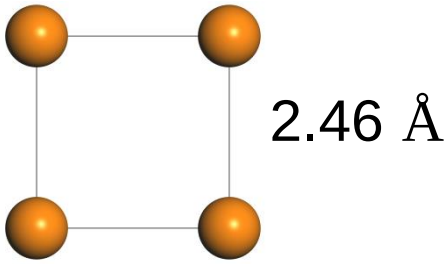
# 11月4日上机实习安排

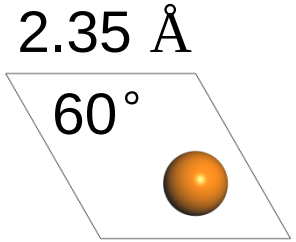
使用MS软件CASTEP模块完成：

Spin-polarized calculation for magnetic Fe membranes:

1. Build slab models for square & triangular Fe membranes
2. **(No Geometry optimizations !!!)** directly perform spin-polarized calculations for different magnetic states
3. Perform spin-polarized calculations for FCC & HCP Fe bulks




FCC(100)_Square Membrane

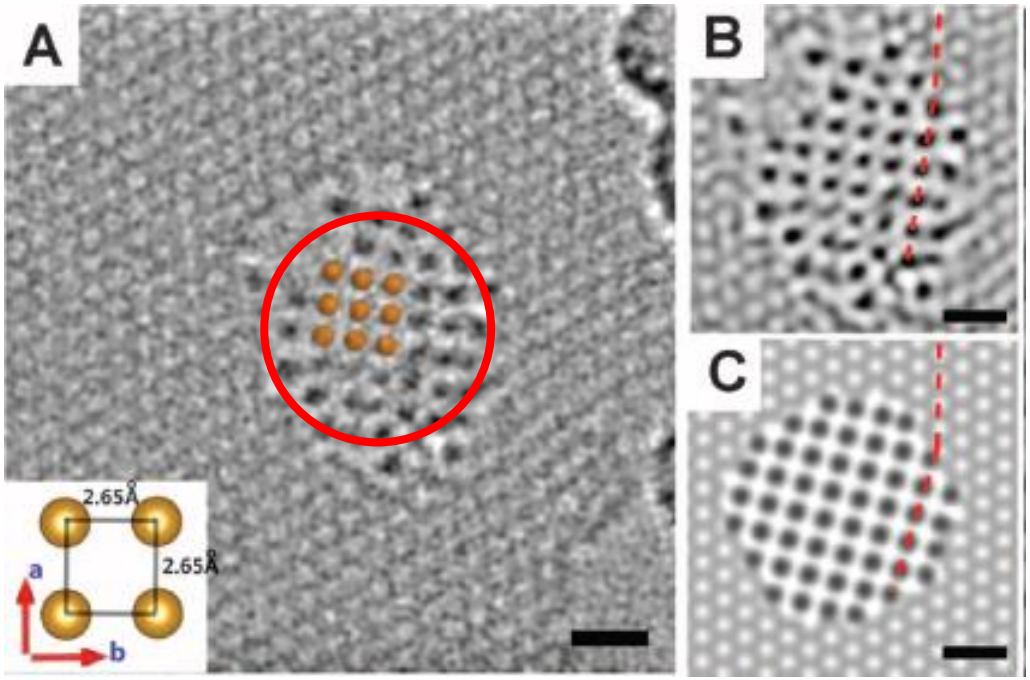



HCP(001)_Rhombic Membrane

# Background of Fe Membranes

- Fe membrane suspended in graphene nanocavity

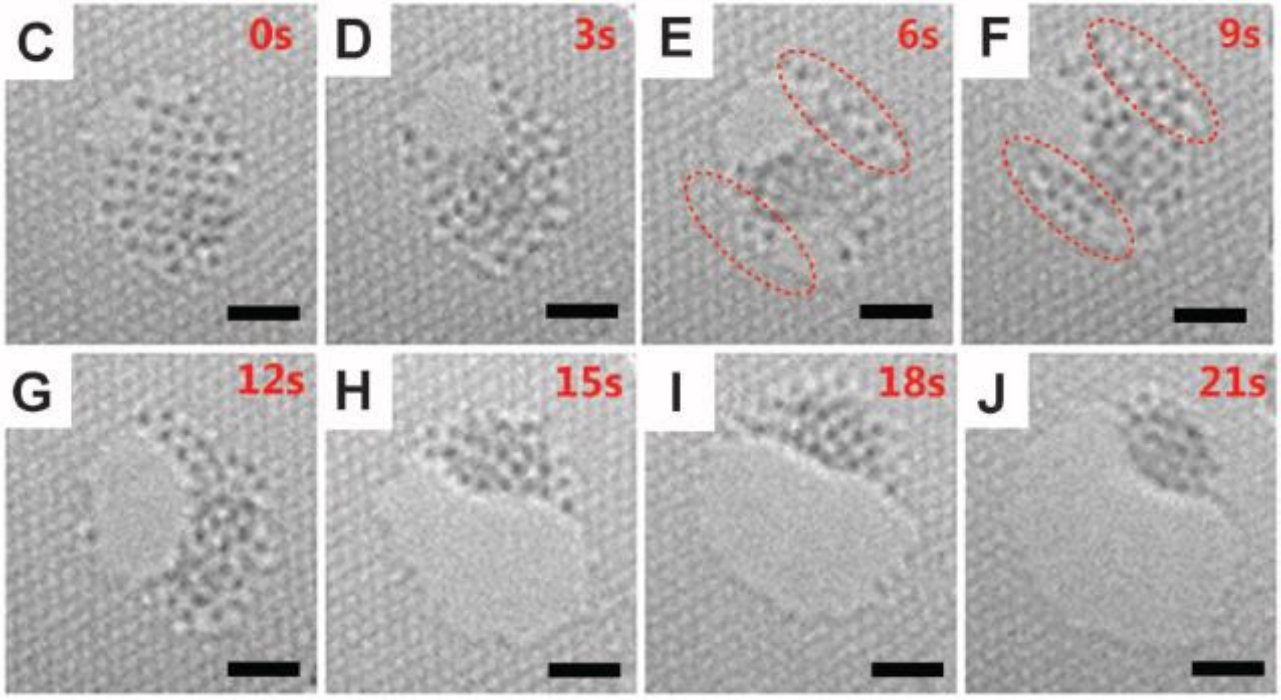
**2D square lattice (2.65 Å)**




*Science* **2014**, *343*, 1228.

# Background of Fe Membranes

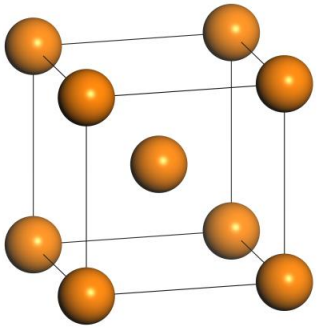
- Collapse of a suspended single-atom Fe layer under electron irradiation



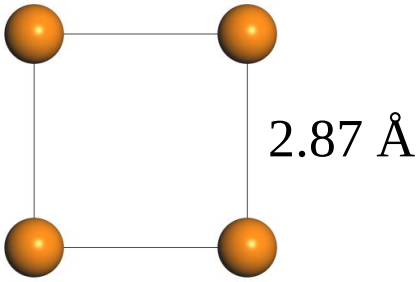

*Science* **2014**, *343*, 1228.

# Reference Structures

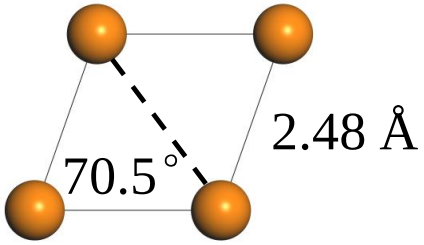
**(a)**



**BCC Crystal**

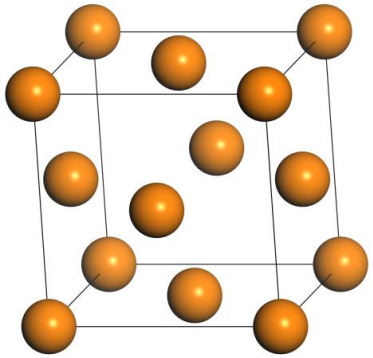



BCC(100)_Square Membrane

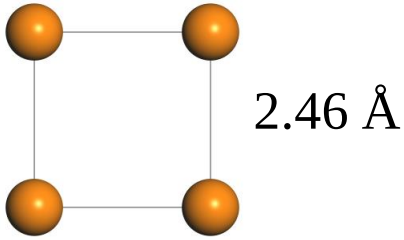



BCC(110)_Rhombic Membrane

**(b)**

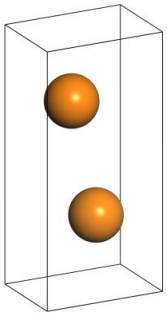


**FCC Crystal**

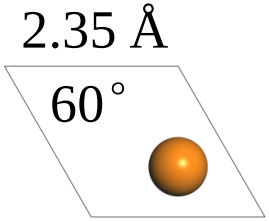



FCC(100)_Square Membrane

**(c)**



**HCP Crystal**



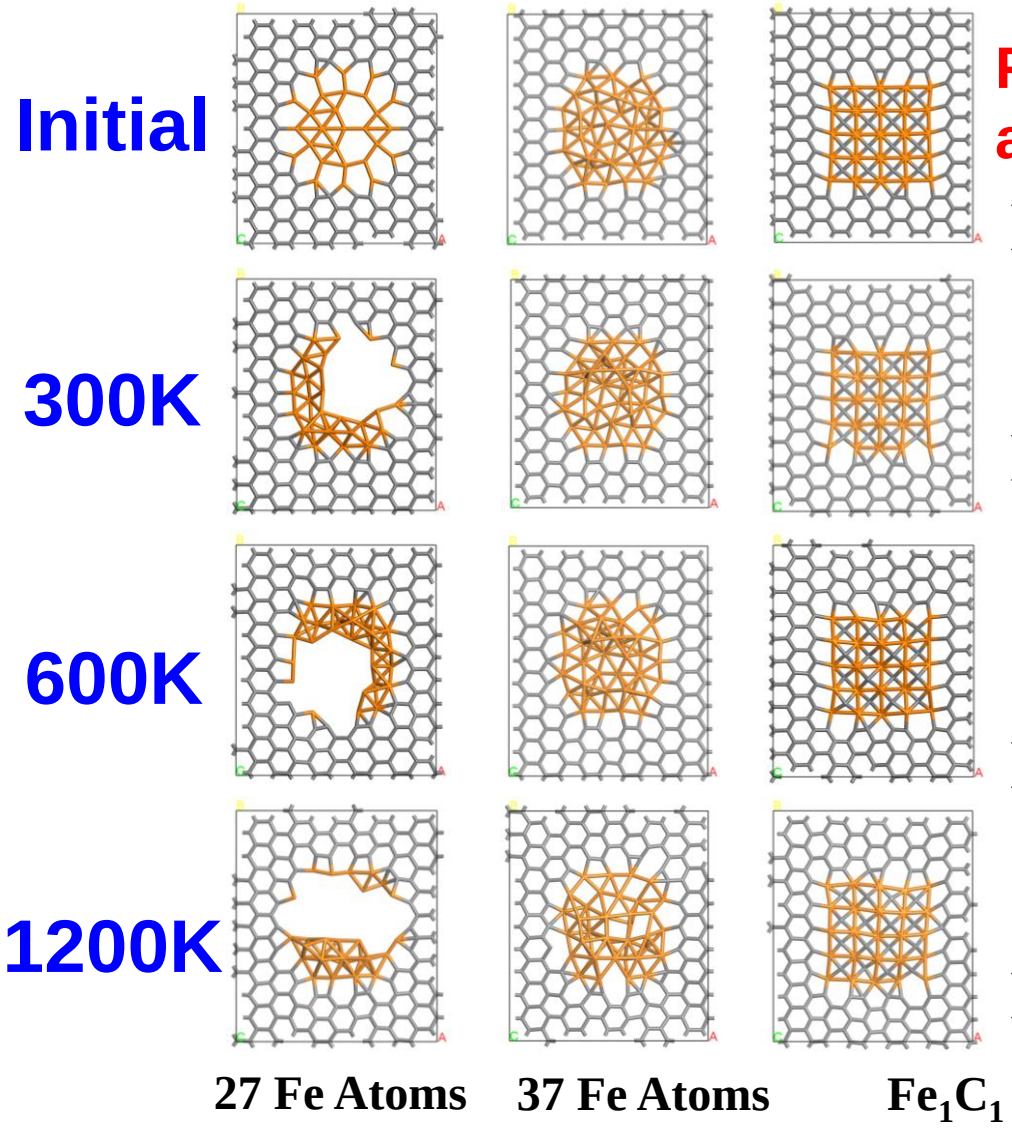

HCP(001)_Rhombic Membrane

**Chen, S.** and Zeng, X. C. *ACS Appl. Mater. Interfaces* **2017**, *9*, 12100.

function (*21*). The calculations show that the in-plane square lattice of monolayer Fe is energetically favored over the other possible 2D configurations, including tetragonal, hexagonal, and so forth. The calculations suggest the most stable lattice constant for monolayer Fe is ~2.35 Å, which is smaller than our experimental value of 2.65 ± 0.05 Å; however, the calculated energy difference between 2.35 Å and 2.65 Å is not large (0.2 eV per atom) (table S1). In addition, some physical aspects not considered in the calculations could lead to a larger lattice constant. For

*Science* **2014**, *343*, 1228.

# Structural Evolution of Fe Nanostructures



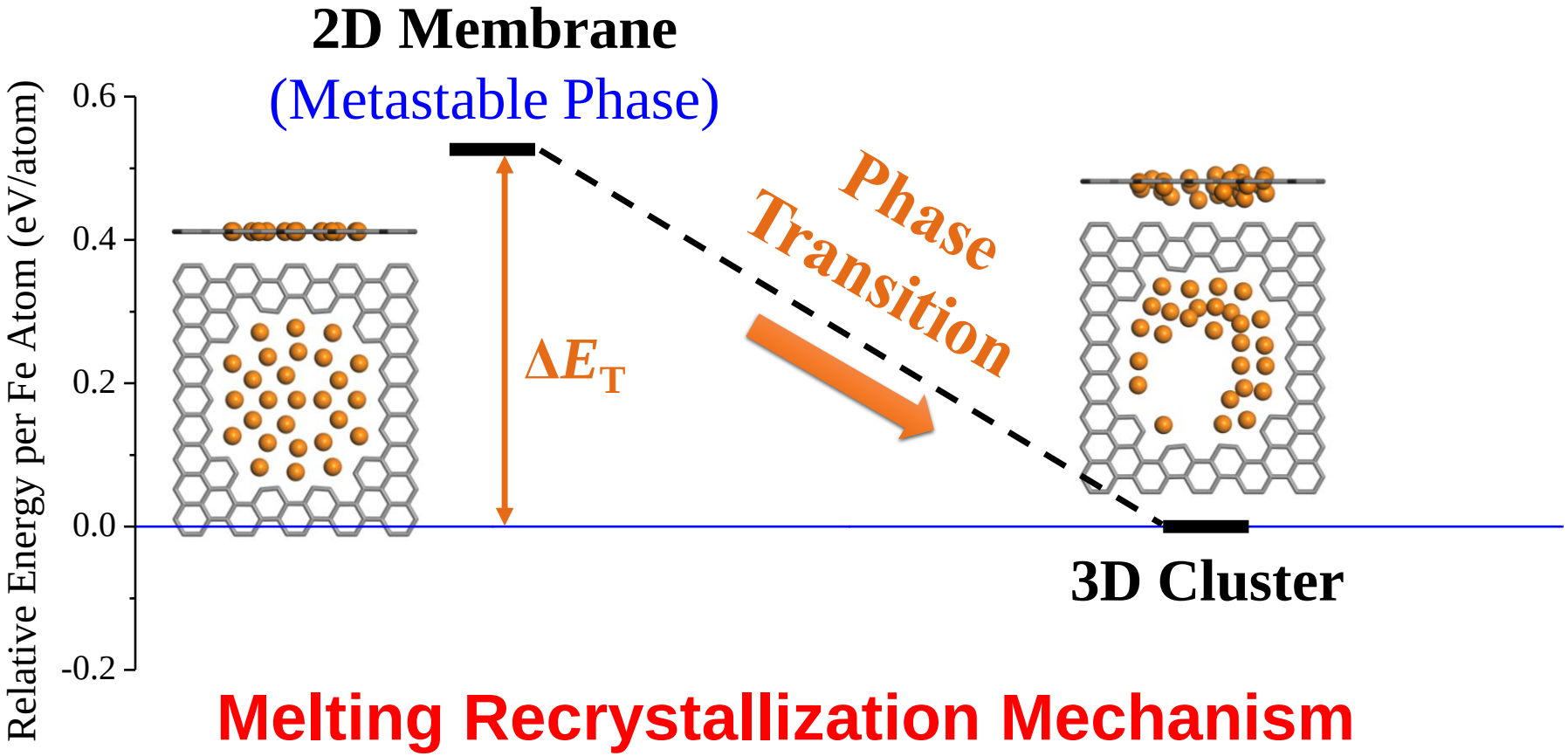

**Fe-Fe bond length: about 2.58 Å**

10-ps AIMD simulations

- Fe atoms seal the graphene nanocavity via growing a metastable Fe membranes.
- The Fe membrane under high tensile strain collapses and turns into a 3D Fe cluster.
- Stability of Fe membranes : densely packed > loosely packed
- Melting recrystallization mechanism

**Chen, S.** and Zeng, X. C. *ACS Appl. Mater. Interfaces* **2017**, *9*, 12100.

# Morphology Change from Metastable 2D Fe Membrane to 3D Cluster




**Melting Recrystallization Mechanism**

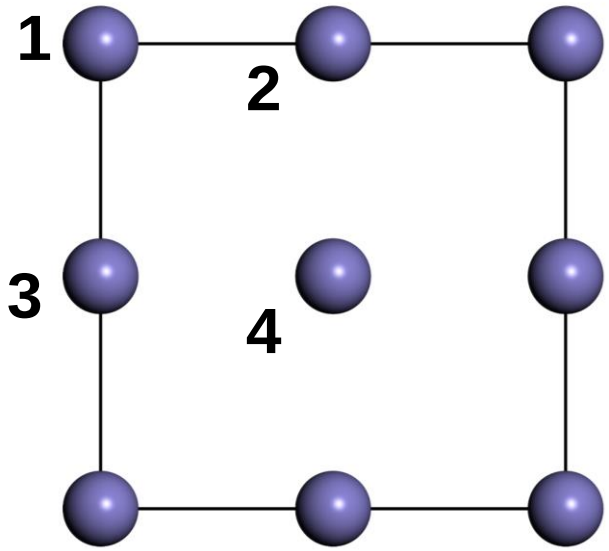
**Chen, S.** and Zeng, X. C. *ACS Appl. Mater. Interfaces* **2017**, *9*, 12100.

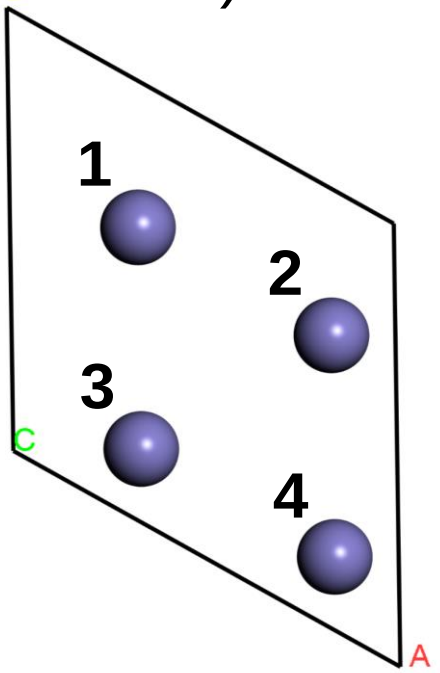
# 1. Build the Slab Models

① Cleave surface along **(100) plane of FCC** Fe bulk (thickness: 0.5) or along **(001) plane of HCP** Fe bulk (thickness: 0.5)

② Add **20 Å**-vacuum layer

③ Build → Symmetry → Supercell (**2×2×1**)

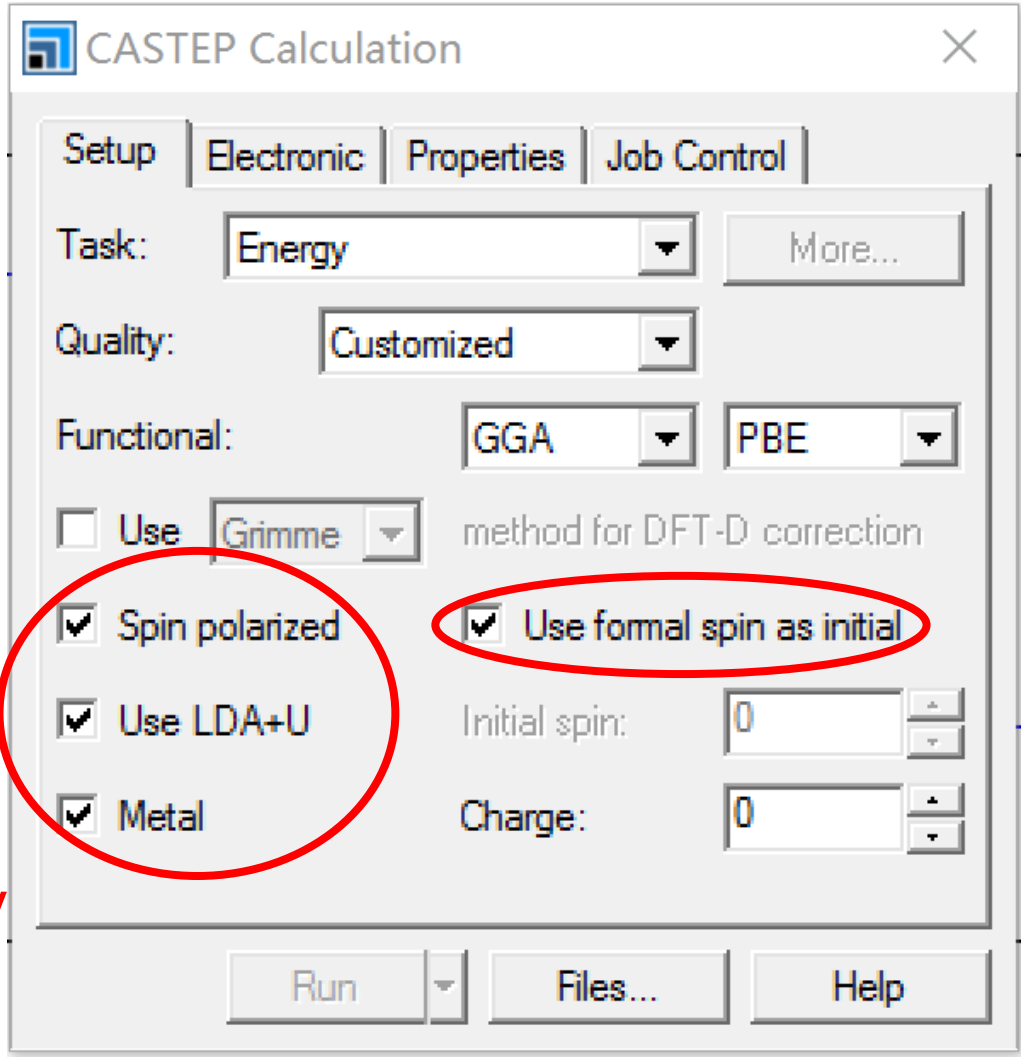


# 2. Magnetic State Calculations

Computational Setting:

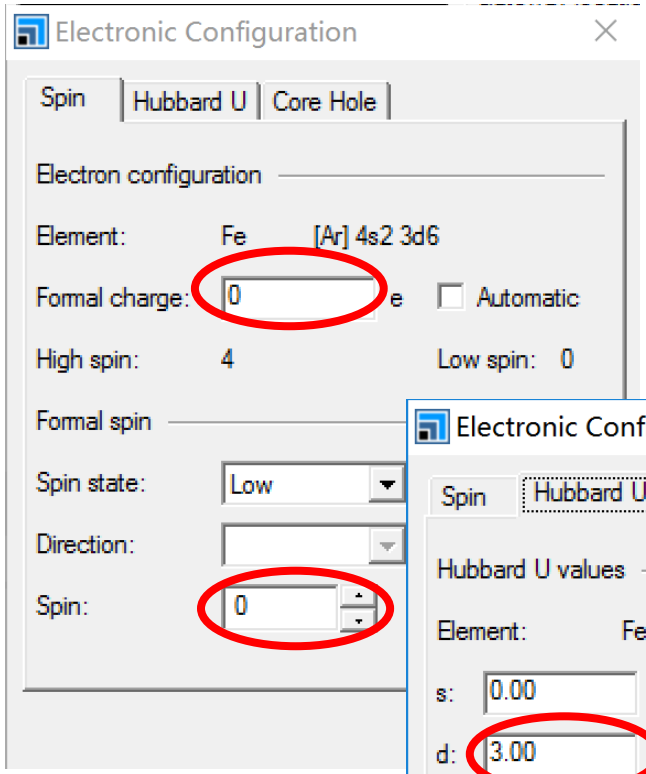
- Method PBE
- Mark “Spin polarized”
- Mark “Use formal spin as initial”
- Mark “Use LDA+U”
- Mark “Metal”
- Cutoff energy: 400 eV
- FFT grid density: standard
- SCF tolerance: 1e-5 eV/atom
- *K* points: Gamma point only

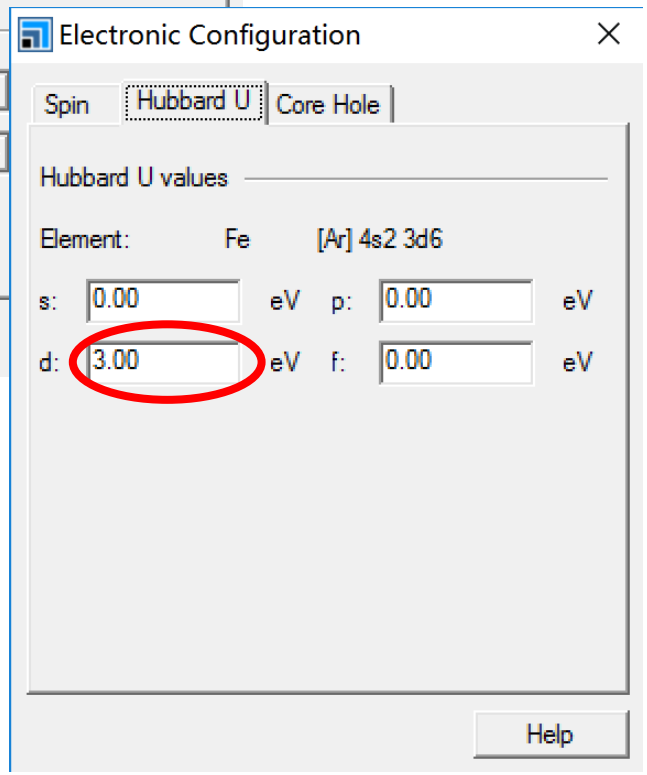


# 2. Magnetic State Calculations

Electronic Configuration Setting for **Ferromagnetic State**:
(Modify → Electronic Configuration)

- Formal charge: 0
- Formal spin: changing from 0 to 4
- Hubbard *U* for *d* orbital of Fe atoms: 3.00 eV

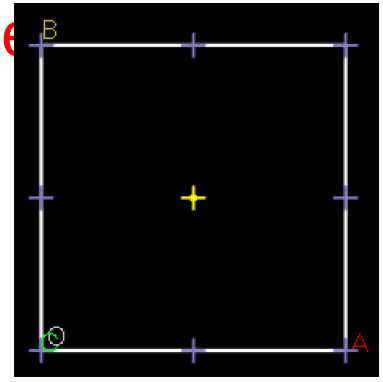


# 2. Magnetic State Calculations

**Magnetic State Switching:**

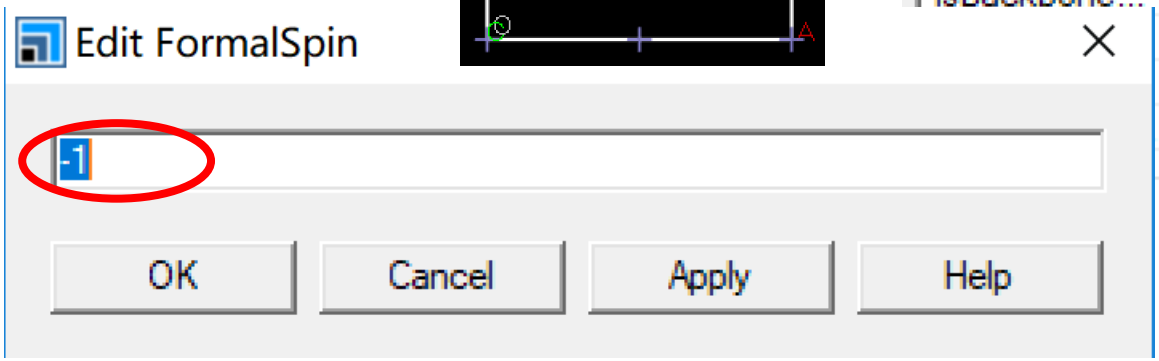
- **In *.xsd window**, select a certain atom
- **In its Properties window**, change its Formal Spin to the specific value




Properties

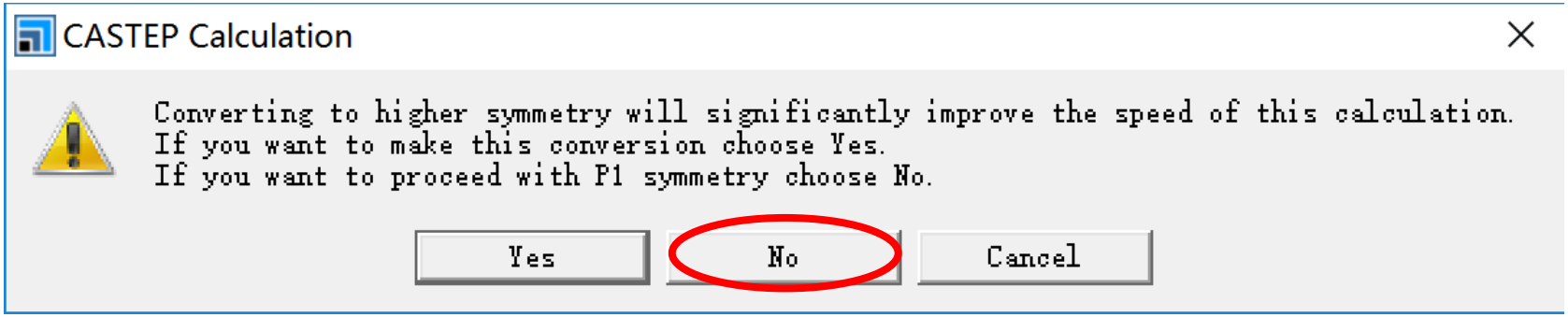
Filter: Atom

| Property | Value |
|---|---|
| Charge | 0.000000 |
| Color | RGB(129, 123, 198) |
| Composition | Fe |
| ElementName | Iron |
| ElementSymbol | Fe |
| ForcefieldType | |
| FormalCharge | 0 |
| FormalSpin | -1 |
| FormalSpinDi... | Down |
| FormalSpinSt... | Custom |
| FractionalXYZ | (0.000000, 0.500000, 1.00000) |
| Hybridization | No hybridization |
| IsBackbone... | No |
| | No |
| | No |
| | No |
| | Yes |



# 2. Magnetic State Calculations

Choose “No” to start the single-point calculations.



# 2. Magnetic State Calculations

- By switching different magnetic states also with different formal spins (from 1 to 4), the energies of Fe membranes with different magnetic states are estimated, learning from *.castep file.
- The one with the lowest energy would be the most possible magnetic state that we search for.
- Compare to the Fe bulks and make conclusion.