Investigation into Structure of Gallium-Selenide Nano Wires

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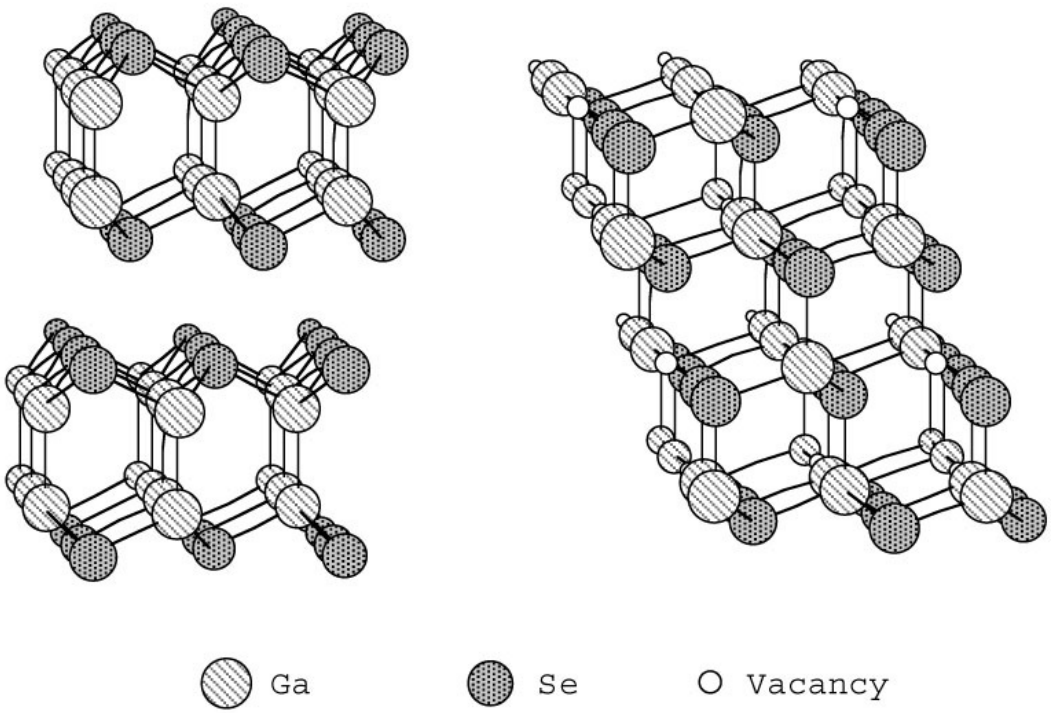
Goals

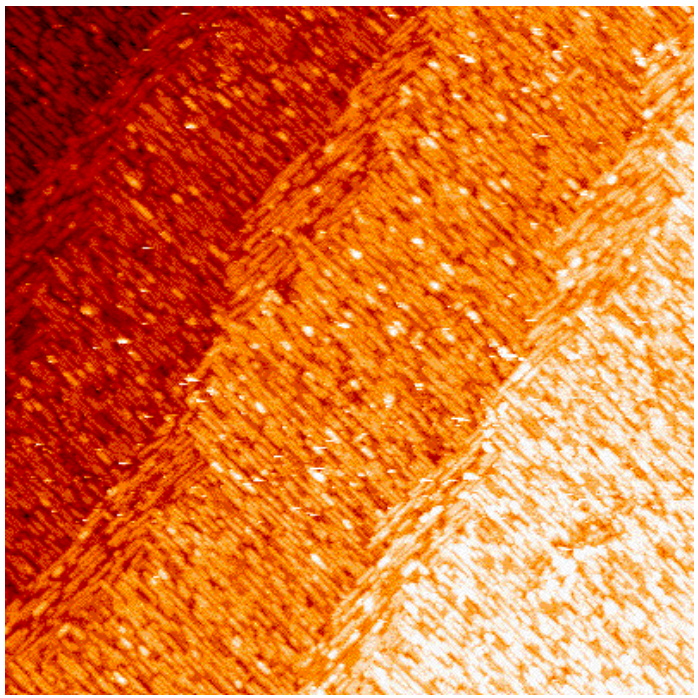
- Primary goal: Determine the structure of gallium-selenide nano wires.
  - Use VASP software to compare energy of different possible structures.
- Short term goal: Calculate density of states for gallium-selenide.
  - Start with silicon, then arsenic terminated silicon.

Ga_xSe_y Observed Structures



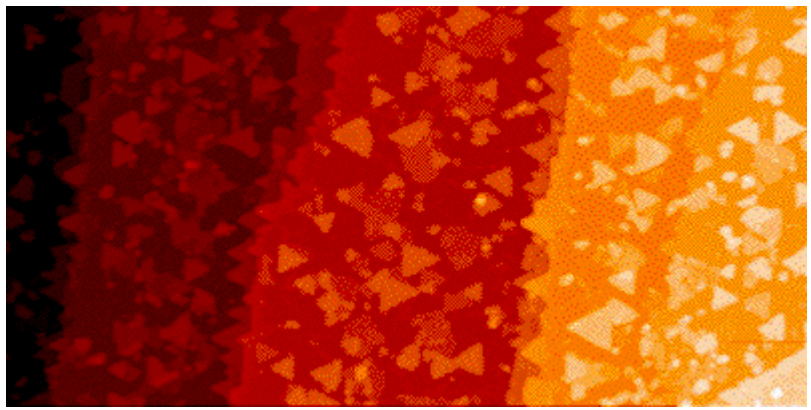
- Two structures observed
  - Layered GaSe (left)
  - Defected zinc-blende Ga_2Se_3 (right)

Ga_xSe_y on Silicon



← 400 nm →

Ga_2Se_3 showing nano wire structure

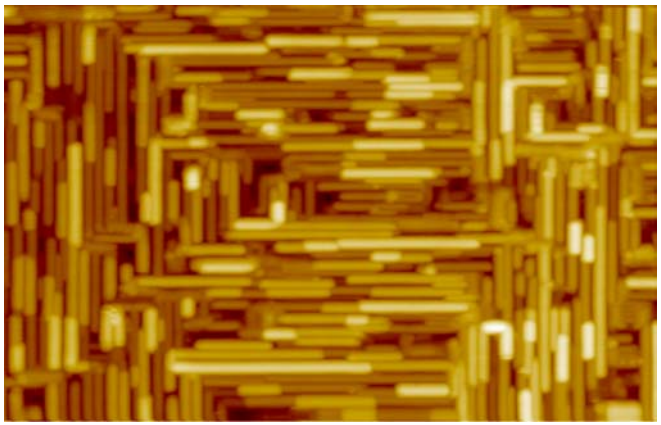


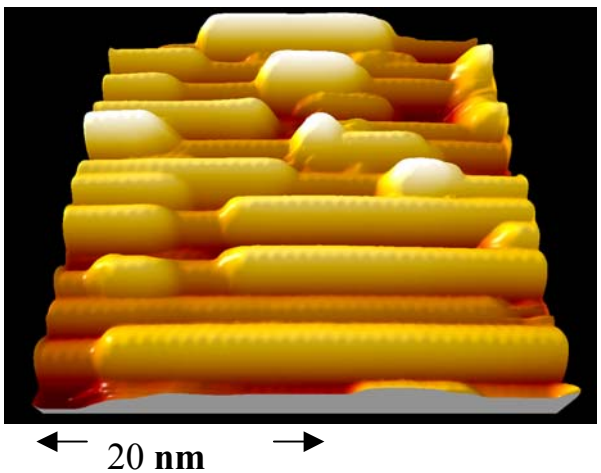
← 350 nm →

Layered GaSe showing cluster structure

(Images taken with scanning tunneling microscope)

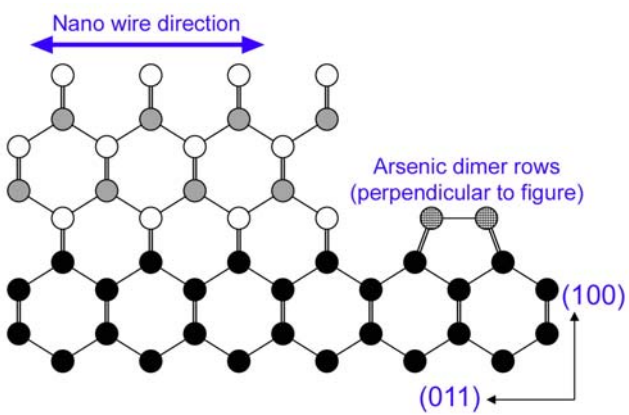
Ga_2Se_3 nano wires

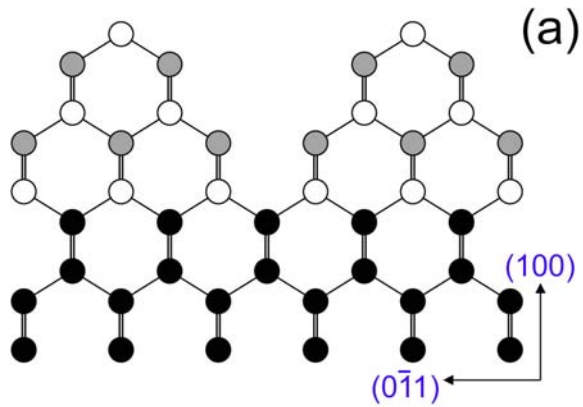




- Structure and growth mechanisms uncertain
- Electrical and optical properties untested
- Could have interesting device applications

Proposed Atomic Structure



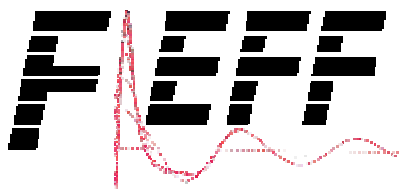


- Wires run perpendicular to arsenic dimer rows
- Gallium atoms on top surface
- Two unit cell spacing

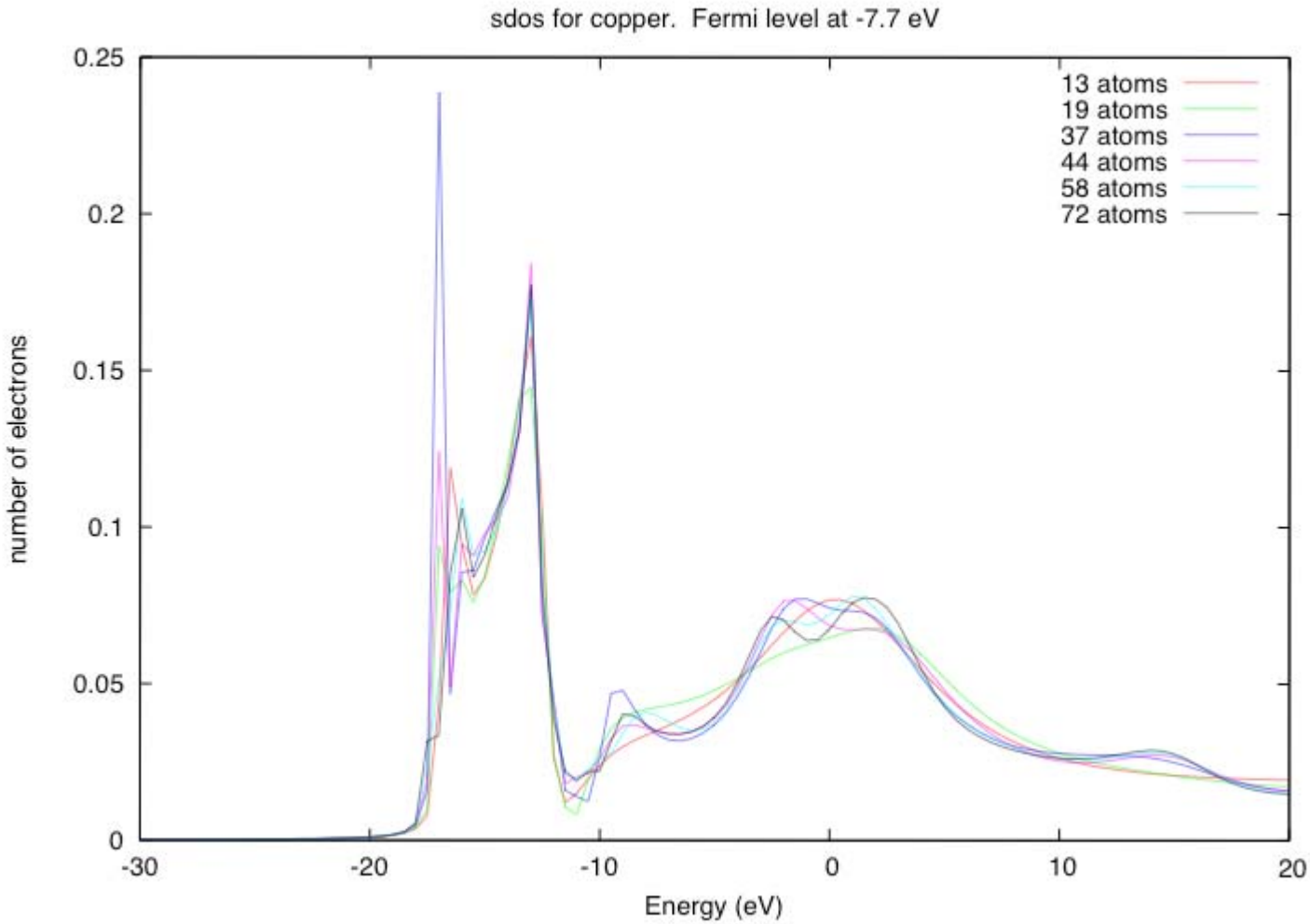
FEFF

Performs *ab initio* calculations of x-ray absorption and electronic structure

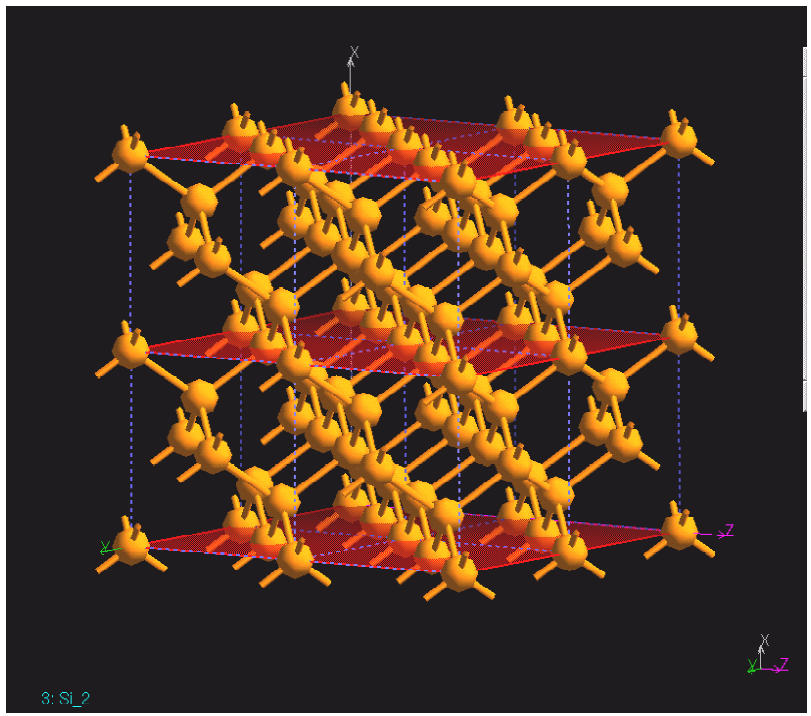
- Used to calculate local density of states (LDOS)
- Works with cluster in real-space
- Self-consistency loop method using atomic potentials



Density of States for Copper



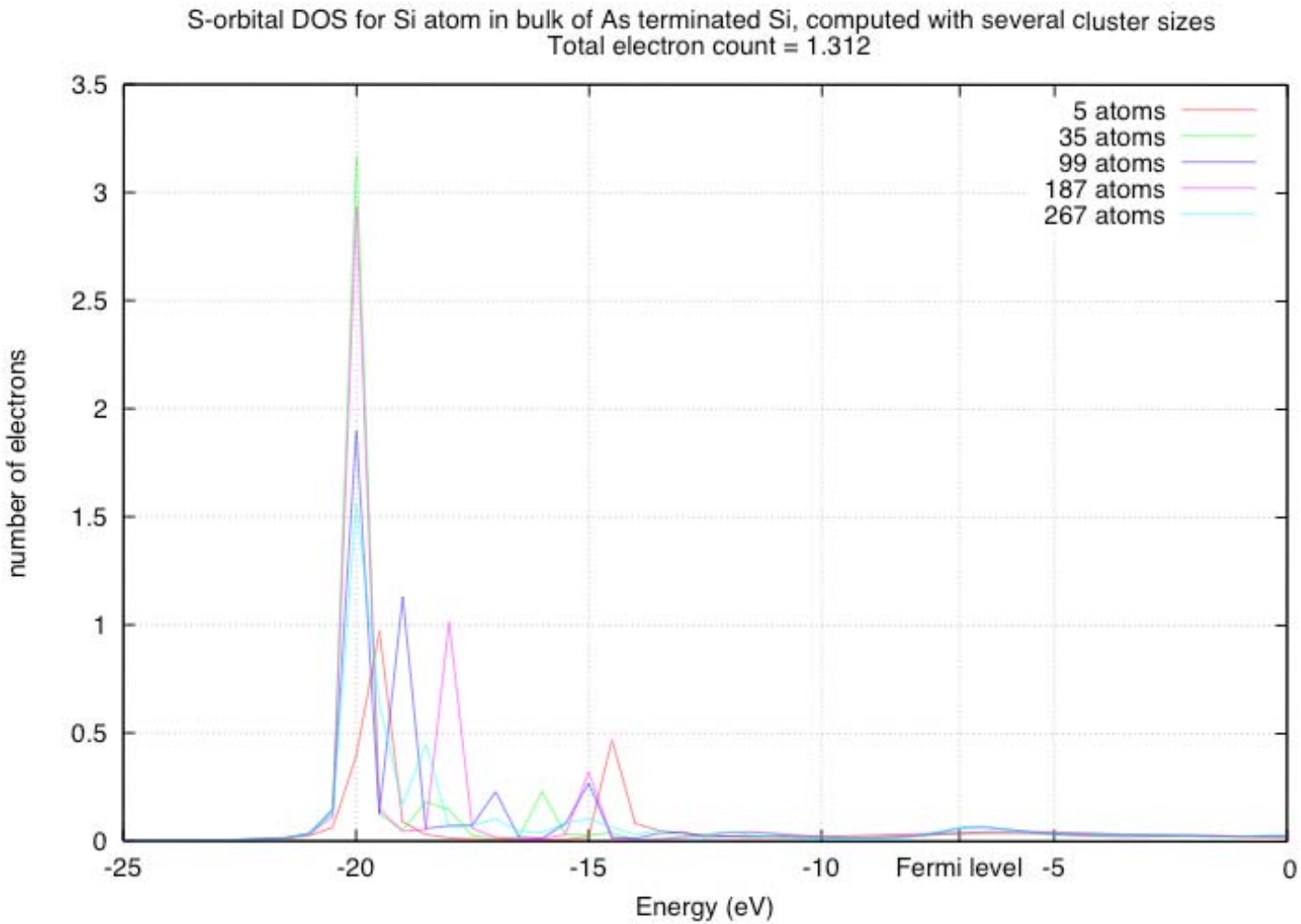
Silicon 100



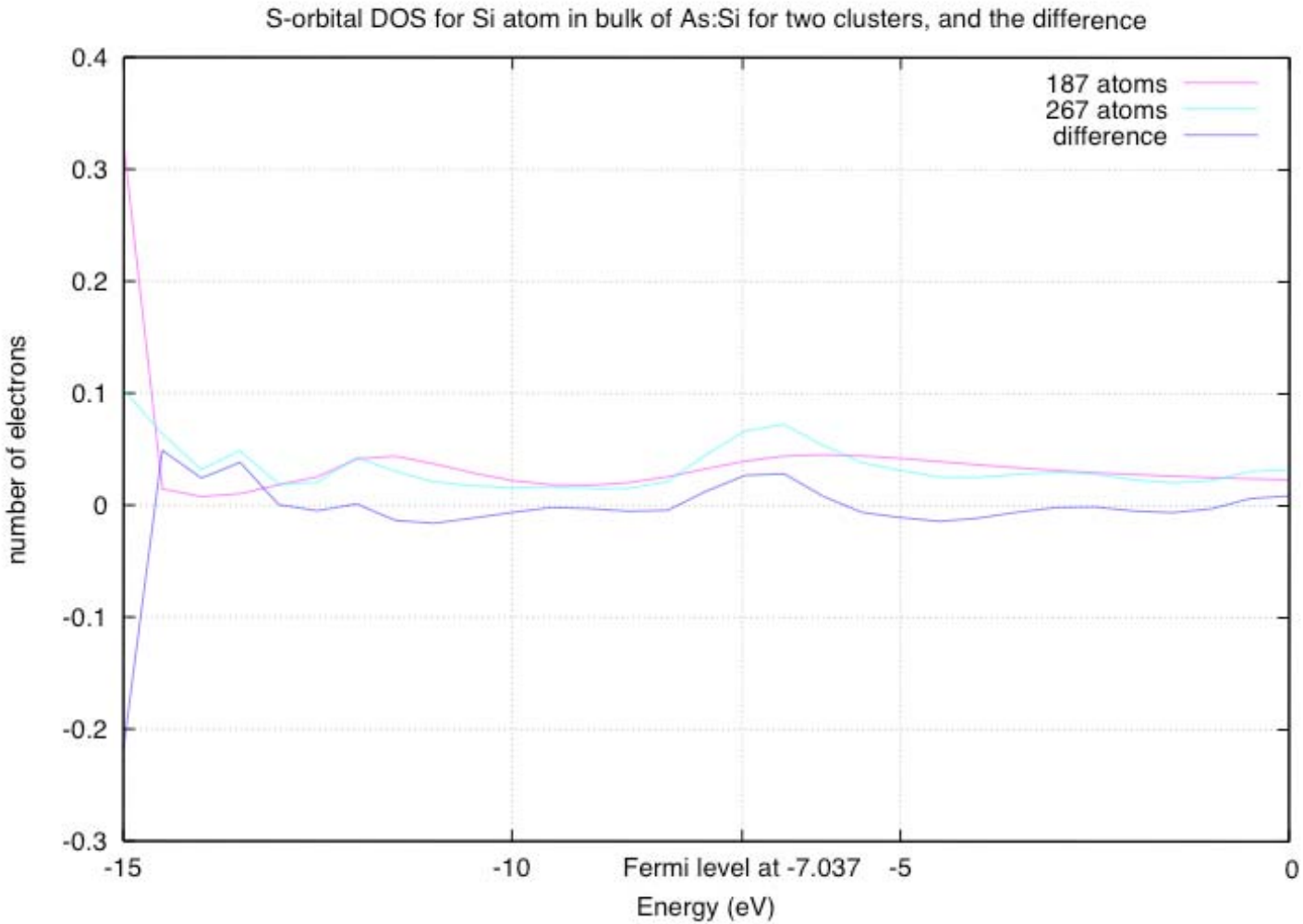
Cluster of eight unit cells of Si 100

- Created model using Cerius (molecule simulation software)
- A little bit of finagling to get it into a Feff input file

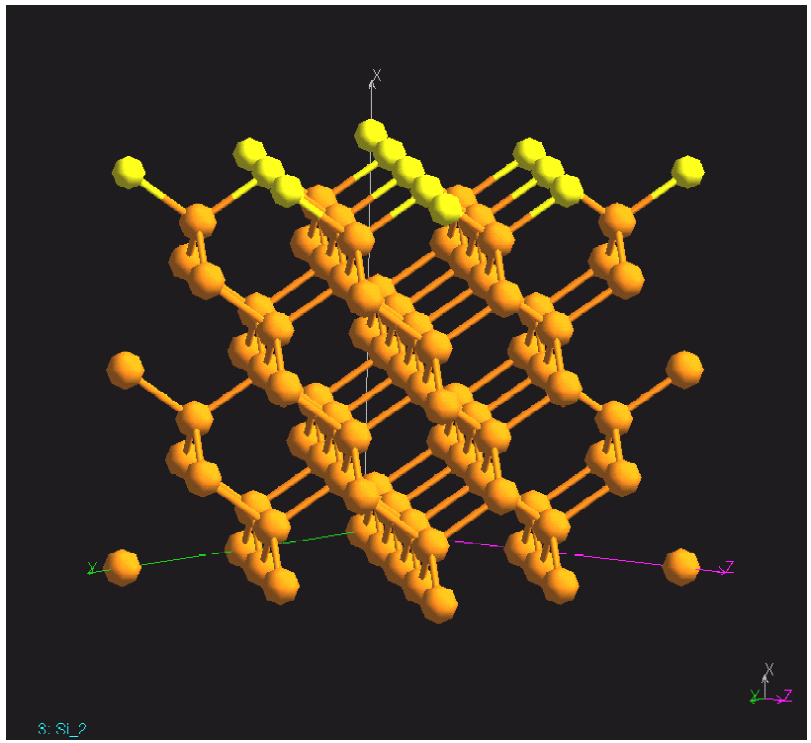
Silicon DOS


S-orbital DOS for Si atom in bulk of As terminated Si, computed with several cluster sizes
Total electron count = 1.312
number of electrons
Energy (eV)
5 atoms
35 atoms
99 atoms
187 atoms
267 atoms
3.5
3
2.5
2
1.5
1
0.5
0
-25
-20
-15
-10
Fermi level
-5
0

Silicon DOS: not yet reached convergence



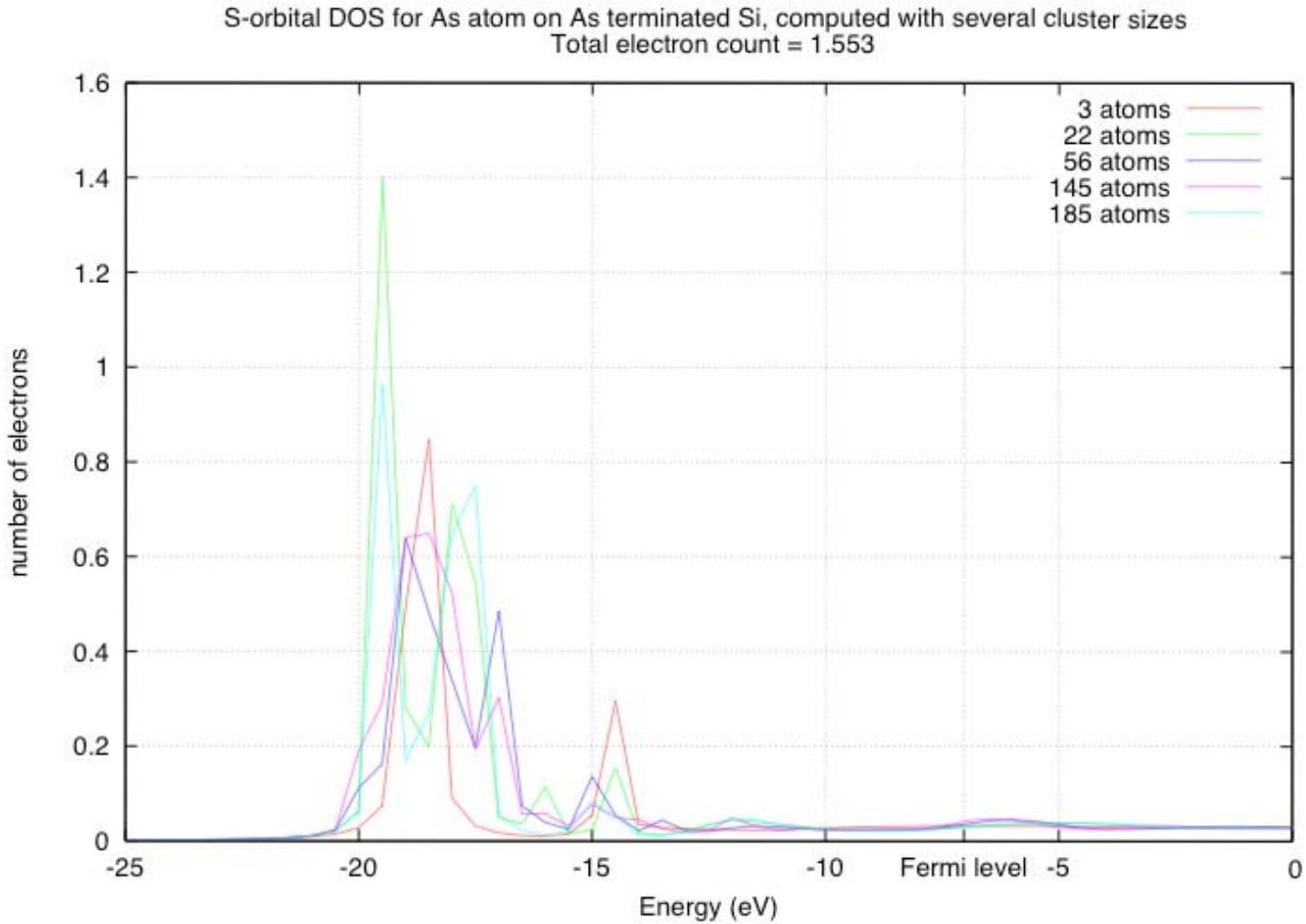
Arsenic terminated Silicon



Cluster of eight unit cells of As:Si

- Model created using Cerius
- Arsenic atoms simply replacing silicon on 100 surface of diamond lattice

Arsenic terminated Silicon DOS

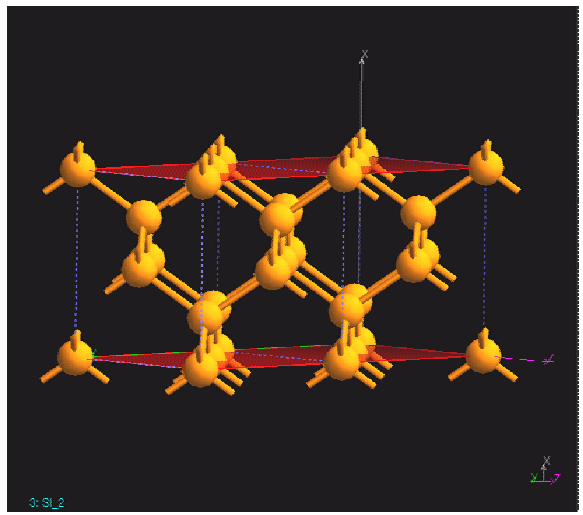


Steps to take for LDOS calculations

- Drastically increase cluster size used in calculations
- Hydrogen terminate the bulk silicon
- Dimerize the arsenic (next slide)
- Add GaSe layer to model

Dimerize the Arsenic

QuickTime™ and a
TIFF (LZW) decompressor
are needed to see this picture.



- Modify model to create dimer pairs between arsenic atoms.
- Re-run FEFF calculations to see if this alters the output significantly.

The next step: VASP

- Performs ab-initio quantum mechanical molecular dynamic
- Works in reciprocal space
- This tool should enable calculation and comparison of energy for possible structures of GaSe.

Conclusions and Future Steps

- FEFF is not well suited to DOS calculation for silicon
- VASP promises better success