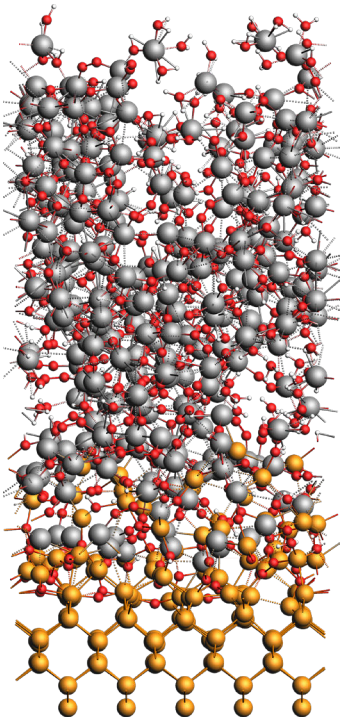
Semiconductors
with the Amsterdam Modeling Suite

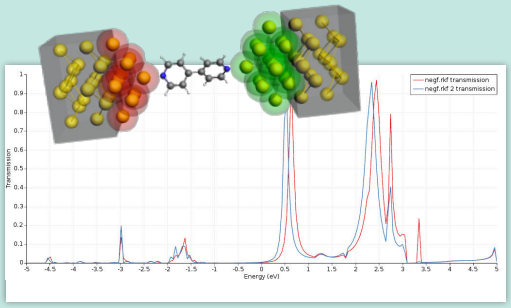
Understand mechanisms and processes, at the atomic scale

As the size of the electronic devices shrink, it becomes increasingly important to understand and predict behavior at the atomic scale. Model molecular systems including nanotubes and nanoribbons, surfaces, bulks, junctions and interfaces to optimize semiconductor materials and processes including vapor deposition, sputtering, etching, nucleation, and crystallization.



What can you compute with AMS?

- Bandgaps
- Electronic transport, effective mass, mobility
- Phonons, thermal transport
- Optical, magnetic, and mechanical properties
- Work functions
- Defect formation energy (neutral and charged)
- Phase diagrams
- Gas-surface processes for deposition and etching

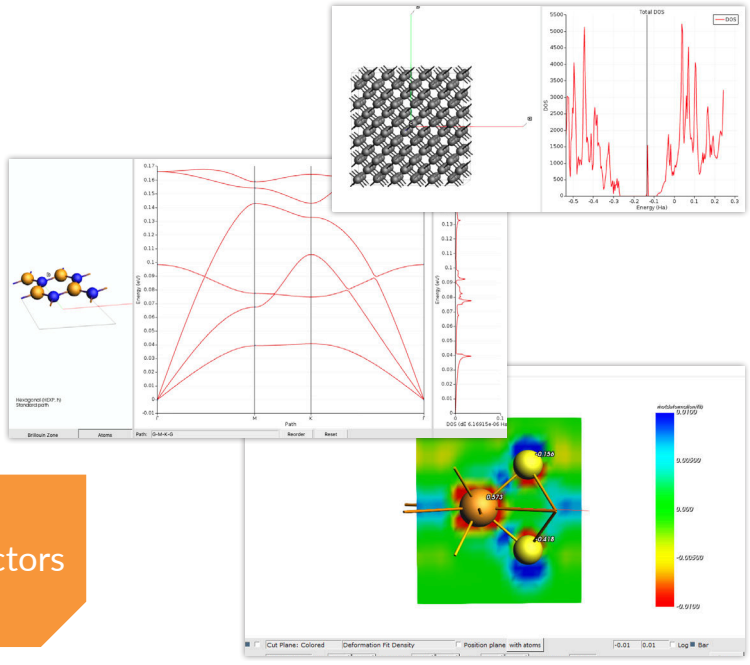


Key methods for semiconductor modeling

- √ Periodic DFT with BAND and Quantum Espresso (QE)
- √ ReaxFF, Machine Learning Potentials
- √ Accurate functionals: metaGGA, hybrids, model potentials
- √ Non-equilibrium Green's function (NEGF) DFT & DFTB
- √ Parametrized DFTB parameters for large scale simulations

Tools and analysis for semiconductor modeling

- Large database of materials
- Crystal, surface, and tube builders
- Graphical user interface for QE and VASP
- Visualize band structures, phonons, DOS
- Field plot tool (planar averaged potential)
- Molecule gun and PES exploration for vapor deposition



SCM
Software for Chemistry & Materials

Explore semiconductors with AMS

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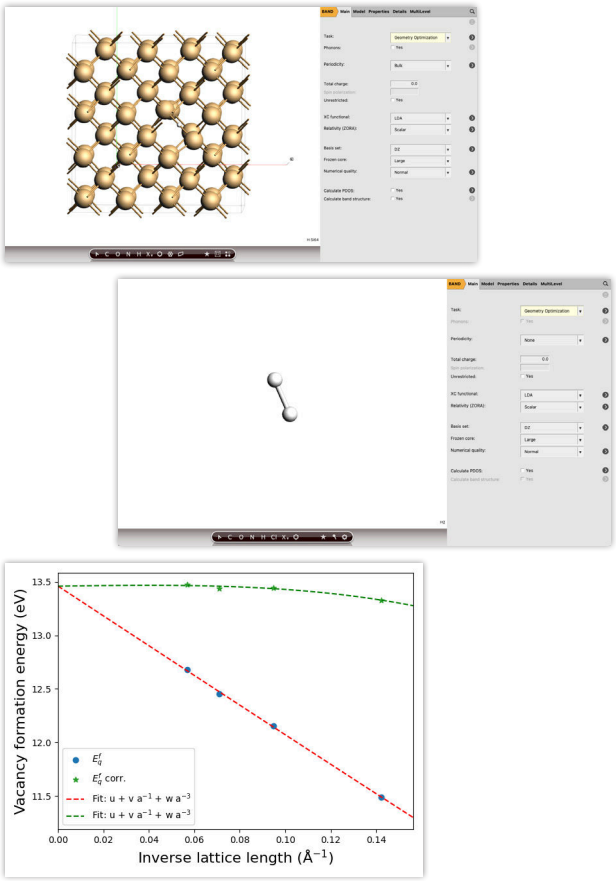
Compute defect formation energy

Point defects are omnipresent in materials and influence their electrical and optical properties. Understanding the formation of defects is critical for many industries in the area of physics and materials science. Therefore, first principles modeling of point defects has become an invaluable tool for understanding materials properties.

Methods and results

Defects can be easily created with the graphical user interface. Load a crystal, interactively delete, move, and create atoms. Define the calculation settings and compute the energy of the pristine and defective materials, as well as the chemical potential of the defect. For charged defects, the spurious long-range Coulomb interaction between supercell images can be corrected using ready-to-use Python workflows.



"What I really like about the Amsterdam Modeling Suite is that the programs were clearly written by chemists for dealing with real chemical problems. A great suite of programs!"

– Roald Hoffmann, Nobel Laureate

About SCM

Scientists at SCM are passionate about making computational chemistry work for you. Our mission is to develop powerful, easy-to-use software for your research and development needs. We love to discuss your research and learn how we can serve you better in the future.

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