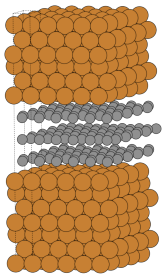
Modelling electronic applications with ASAP

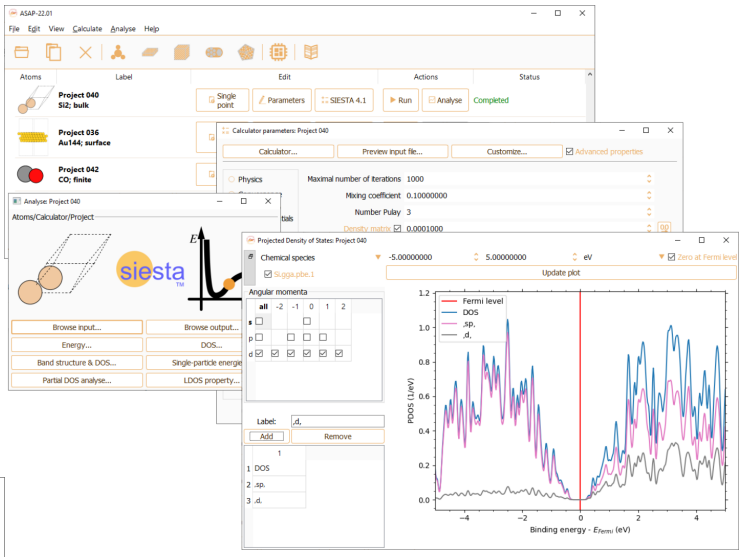
Miniaturisation of electronic components has led to creation of portable computer devices. **Modern electronics industry** has already employed recent **nanometers** MOSFET technologies. At such a scale knowledge of the atomic structure and electronic properties become essential for the design and performance of nanoscale electronic devices. Such properties of materials can be routinely studied using modern methods of quantum physics using computer modelling.

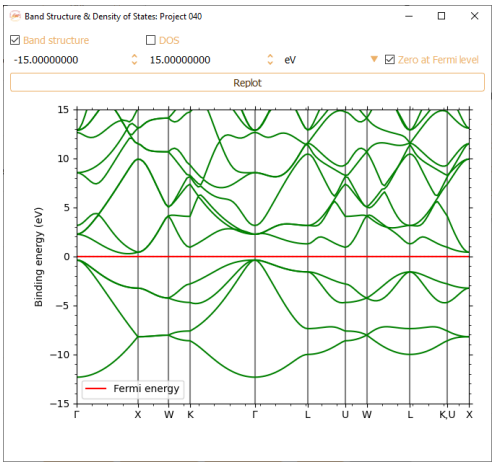


Advanced Simulation Atomistic Platform (**ASAP**) is a powerful software solution for advanced modelling of electronic devices. ASAP facilitates the design of complex structures due to its powerful structure builder and editor widget. ASAP allows users to intuitively construct complex structures: Upload molecular structures from ASAP databases, create a bulk material using the most common crystal structures, generate surfaces with arbitrary orientation, construct supercell slabs and build single-walled nanotubes. Structures can be merged to construct complex interfaces between built surfaces and/or molecular materials.

ASAP computes relevant electronic properties essential for modelling **electronic devices**:

- ➔ Optimal material geometry
- ➔ Total and Fermi energy
- ➔ Electronic level energies
- ➔ Band structure
- ➔ Total Density Of States (DOS)
- ➔ Partial DOS
- ➔ LDOS





ASAP employs the **SIESTA** code for quantum mechanical calculations, the code, well known for its excellent performance tackling computationally demanding systems (>10000 atoms).

ASAP has a range of robust post production and visualisation tools that severely simplify the analysis of the electronic properties of semiconductor devices.

SIMUNE is an expert in atomistic quantum mechanical simulations for electronic applications. SIESTA case study for semiconductor applications can be found at the SIMUNE web-page.

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