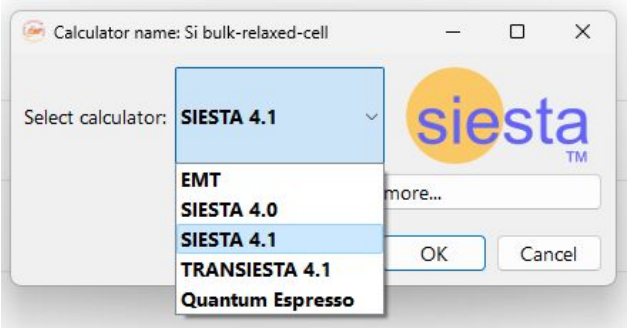
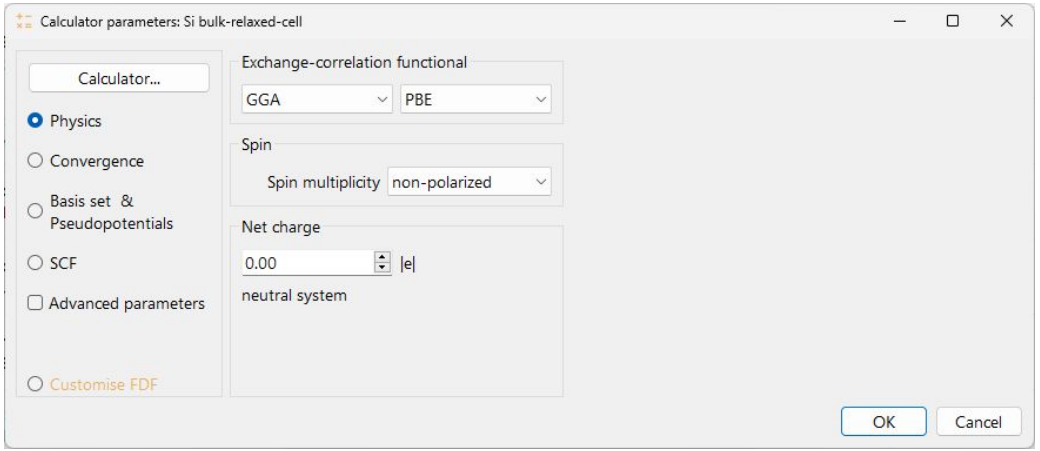
Computing Si bulk properties with ASAP Solvers

Calculator: Solvers within ASAP

Within ASAP, the Graphical User Interface designed to assist users in selecting the computational engine and properly preparing the input file is named “The Calculator”.

ASAP Calculator supports various solver engines





Common features:

- Code parameters organized into intuitive categories
- Initial parameters suggested
- Advanced settings

Calculator: Solvers within ASAP

What is the most suitable solver for my calculations?

- **EMT** (Effective Medium Theory). Only for test and demonstration purposes

- **SIESTA** (DFT / basis set: Linear Combination of Atomic Orbitals / pseudopotentials)
  - Can treat: periodic, finite and open systems (slabs, surfaces, clusters, nanotubes and molecules)
  - Best performance for computationally demanding systems
  - Tunable performance

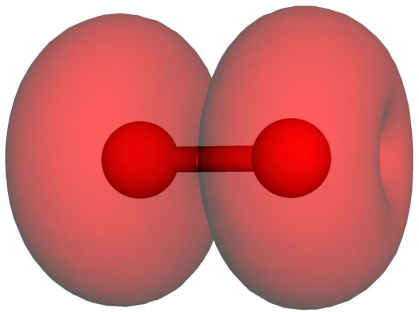
- **Quantum Espresso (QE) (**DFT / basis set: Plane Waves /pseudopotentials)
  - Can treat: periodic, finite and open systems
  - High precision (non tunable)
  - Hybrid functionals

- **TranSIESTA** (NEGF / basis set: Linear Combination of Atomic Orbitals / pseudopotentials)
  - Can treat: open system formed by a finite structure sandwiched between two semi-infinite metallic leads. A finite bias can be applied between both leads, to drive a finite current. Output: transmission and I-V curve

Calculator: Solvers within ASAP

Atomic orbitals and planewave are two of the main types of basis set used to describe the molecular orbitals

Molecular orbitals



Atomic Orbitals:
localized functions centered on atoms

siesta™

- Accuracy and cost can be tuned from quick exploratory calculations to highly accurate simulations.
- Maintains an advantageous computational cost compared to other methods.

Plane Waves:
delocalized functions that extend throughout the entire simulation cell

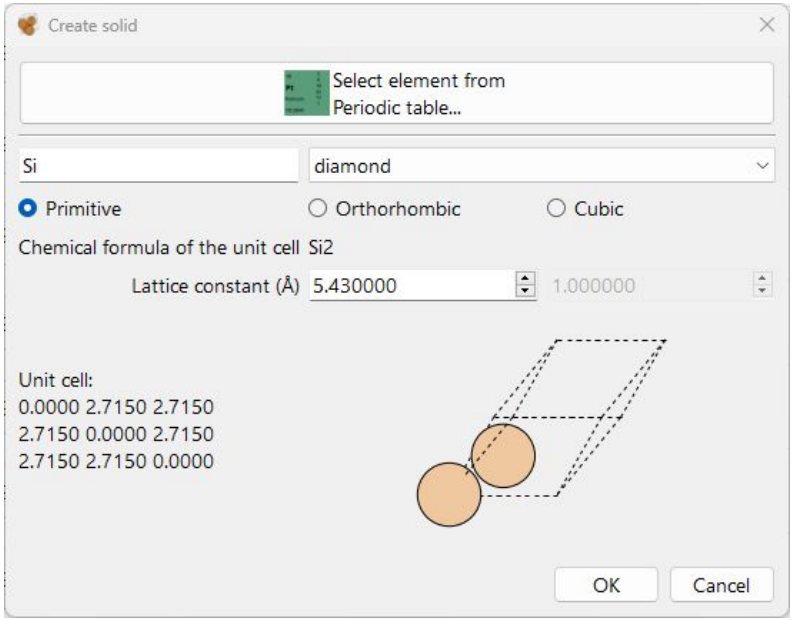
QUANTUMESPRESSO

- Consistently high accuracy systematic convergence
- Generally requires higher computational resources

Comparing performance of ASAP Solvers

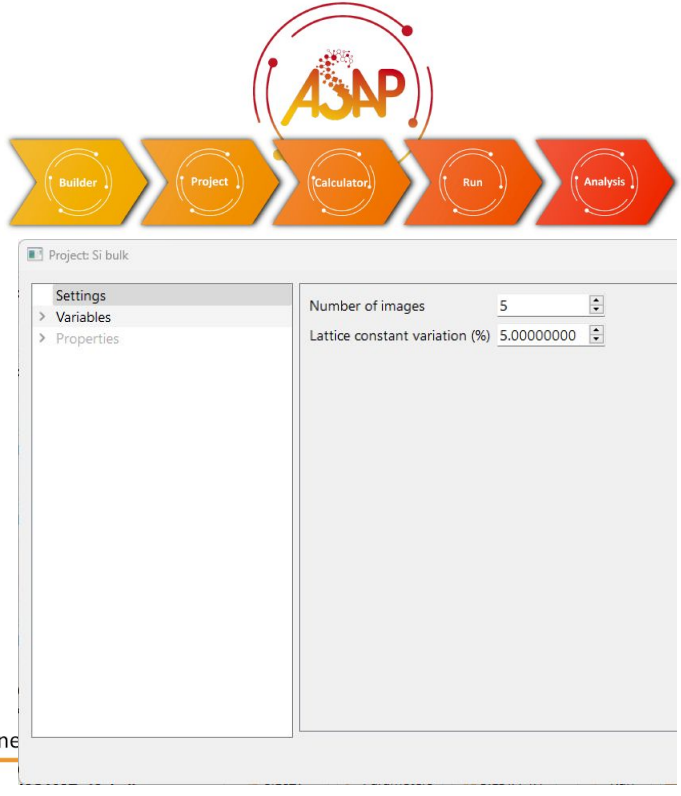
In this case study, we compare the performance of the ASAP solvers, SIESTA and Quantum Espresso, in predicting the lattice constant and the bulk modulus of silicon (Si) bulk.

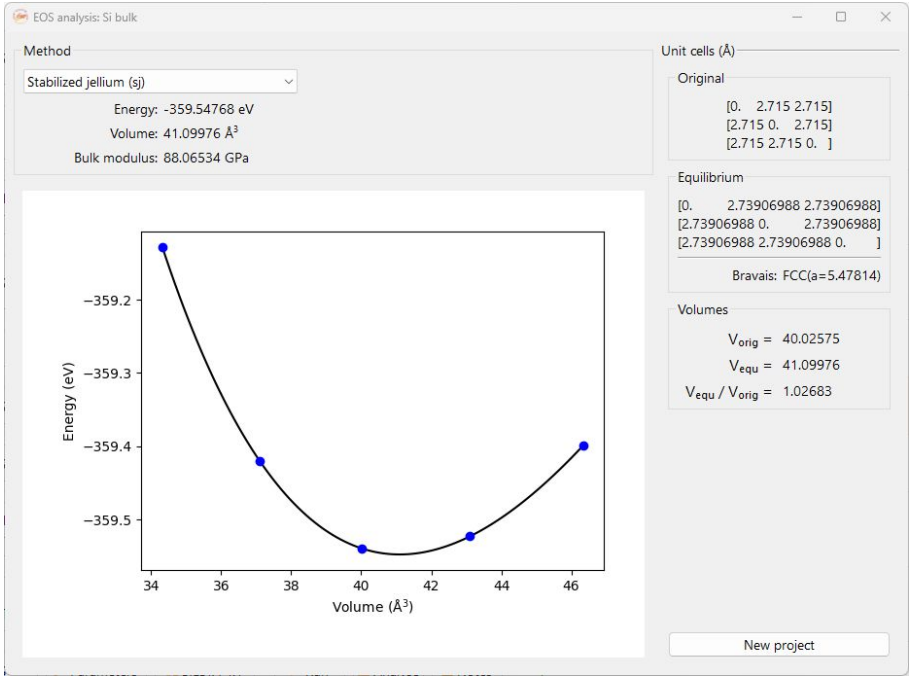
We easily create the crystal structure with ASAP builder



Comparing performance of ASAP Solvers

A series of single-point calculations are carried out to compute the ground-state energy for different lattice constants using an automated workflow in ASAP (Equation of State)





Comparing performance of ASAP Solvers

The Si cell parameter computed by SIESTA is in reasonable agreement with that computed by QE. Both slightly overestimate the experimental cell parameter (approx. 0.87% and 0.74%, respectively). This overestimation is known to occur with GGA functional.

Bulk Si	SIESTA[1]	QE[2]	Exp[3]
a (Å)	5.478	5.471	5.431
B (GPa)	88.1	88.5	98.74

[1] SIESTA Calculator (4.1). PBE. Basis set optimised by SIMUNE based on the minimization of the average energy of a dimer system with different interatomic distances. https://www.simuneatomistics.com/siesta-pro/siesta-pseudos-and-basis-database/
[2] Quantum Espresso Calculator, PBE. ecutwfc = 30.0, ecutrho = 200.0
[3] https://www.matweb.com/search/DataSheet.aspx?MatGUID=7d1b56e9e0c54ac5bb9cd433a0991e27&ckck=1

Request a trial version of ASAP.

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