Atomistic Simulation Advanced Platform

A. Kimmel, A. García, P. Koval, I. Lebedeva, F. Marchesin, Y. Pouillon, M. García-Mota

SIMUNE Atomistics, Tolosa Hiribidea 76, Donostia-San Sebastián 20018, Spain

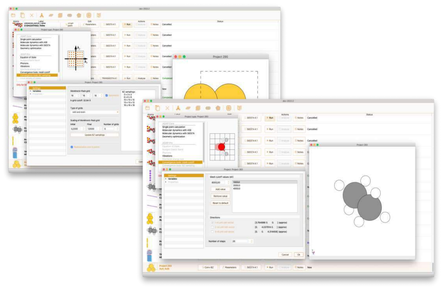
commercial@simuneatomistics.com

SIMUNE Atomistics is a scientific software manufacturing company producing scientific software solutions based on quantum mechanical and atomistic approaches for semiconductor, automotive, chemical and green energy industries.

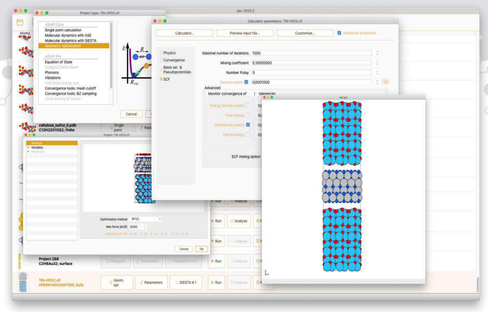
ASAP -- Atomistic Simulation Advanced Platform -- [1] is **SIMUNE's product** devoted to creation, steering and analysis of atomistic calculations. It includes powerful structure builder, several algorithmic workflows, local and remote calculations control, and comprehensive tools for results analysis.

FUNCTIONALITY

- Cross Platform performance: Linux, Mac, Windows
- Ready to use: installation package with libraries and solvers supplied
- Interactive GUI: Flexible intuitive widgets for visualisation, job control, post analysis
- Local and remote run: Flexible set, data acquisition from remote HPC facility
- Extended terminal
- Powerful solvers: SIESTA, EMT



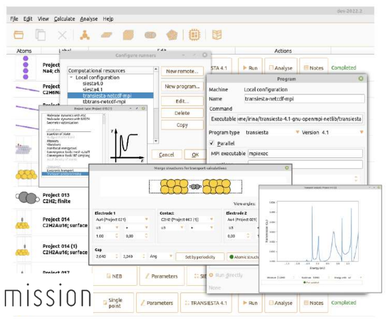
STRUCTURE BUILDER



- Built-in molecule library
- Library of common crystal structures
- Bonds, distances, angles measurement
- Custom slab surface cut
- Nanoparticle and nanotube builder
- Import /export structures to various output formats
- Dynamic visualisation: animation, rotation, translation
- Structure manipulation: select, add, delete, modify atoms/ selection
- Merge structures, modify cell parameters.

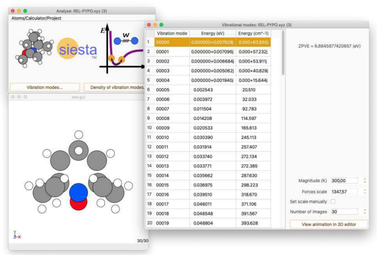
WORKFLOWS

- Input Parameters Convergence
- Single Point and Geometry
- Optimisation
- Molecular Dynamics
- Electron Transport
- Interfacial Energy
- Nudged Elastic Band
- Equation of States
- Molecular Vibrations
- Phonons



ELECTRONIC TRANSPORT

- Device builder
- Zero/non-zero bias transmission
- Current-voltage characteristics
- Electrode transmission and Density of States
- Transmission eigenvalues and eigenstates
- Projected transmission
- Orbital current



PHONONS AND VIBRATIONS

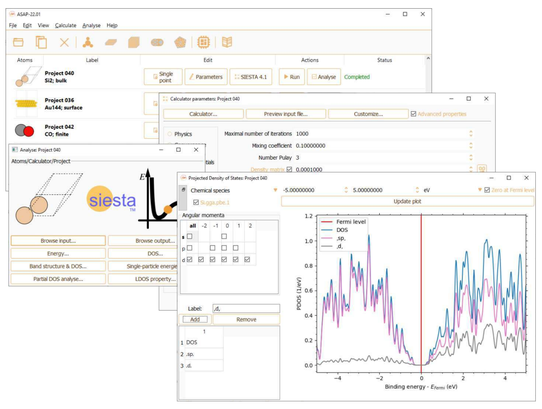
- Phonon density of states
- Phonon band structure and density of states
- Edit Band path
- Zero-Point Energy Correction (ZPVE)
- 3D visualisation of molecular vibration

GEOMETRY OPTIMISATION AND MOLECULAR DYNAMICS

- Visualisation of optimised geometry and steps
- Visualisation of structure evolution during the MD run
- NVE and NPT (ASE)
- NVE, NVT, NPT (SIESTA)
- Visualisation of time series
- Kinetic, Potential, Total Energies
- Temperature Evolution
- Pressure Evolution
- Radial Distribution Function

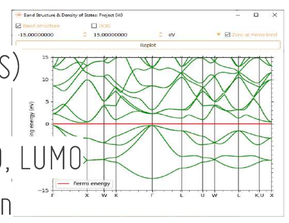
ASAP- for electronic industry

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



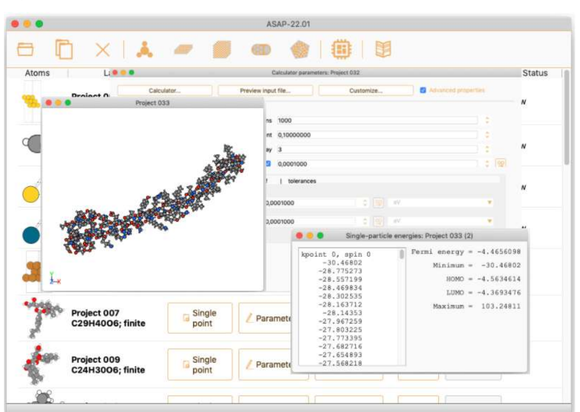
The platform computes a range of electronic properties essential for modelling devices:

- Fermi energy
- Band Structure
- Band structure visualisation, path definition/edition
- Density of States (DOS)
- Partial Density of States (PDOS)
- Charge Analysis
- Single Particle Energies: HOMO, LUMO
- Molecular Orbitals visualisation



ASAP- for bio-chemical applications

ASAP provides a powerful environment for large-scale atomistic simulations of bio-matter. The platform enables to construct, and visualise complex bio-models thanks to powerful structure builder and flexible molecular editor widget.

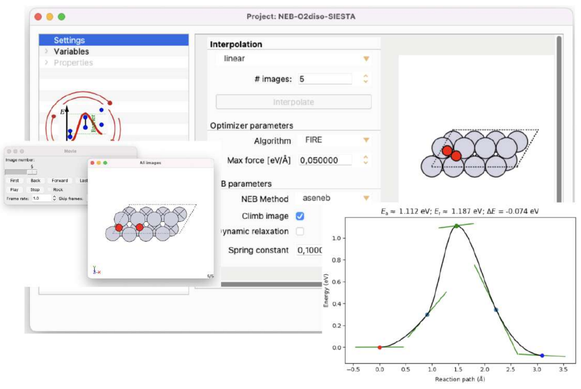


ASAP employs the **SIESTA** code [2-4] well known for its excellent performance for computationally demanding systems over 10^4 atoms.

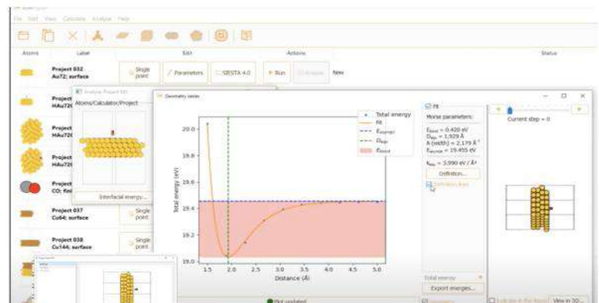
The platform brings powerful capability for modelling of bio-systems with explicit solvent, efficient post-production tools to analyse structural, chemical, electronic and dynamic properties of simulated systems.

ASAP – for catalytic applications

ASAP provides a powerful environment for catalysis workflows. The platform has a robust structure builder that facilities the set up of catalytic material, upload molecules from an extended database, create crystal structure, build a surface with arbitrary orientation and elements, construct single-walled nanotubes, estimate reaction energies and barriers, calculate vibrational properties, zero-point energy corrections.



Nudged Elastic Band (NEB) tool implemented in **ASAP** makes it a powerful instrument for modelling chemical reactions and catalytic processes, enabling characterisation of the minimum energy reaction path and transition states.



Interfacial Energy Tool (IET) is a robust instrument for modelling complex interactions between molecules and interfaces. The tool enables automatic parametrisation of interaction energy in the form of analytical potential for semiempirical calculations.

References

[1] F. Marchesin, P. Koval, Y. Pouillon, I. Lebedeva, A. García, M. García-Mota, A. Kimmel "Atomistic Simulation Advanced Platform (ASAP) for materials modelling with ab initio methods", Psi-k conference 2022, Lausanne (Switzerland).

[2] E. Artacho, D. Sánchez-Portal, P. Ordejón, A. García, J.M. Soler, Linear-Scaling ab-initio Calculations for Large and Complex Systems. phys. stat. sol. (b), 215: 809-817 (1999).

[3] E. Artacho, E. Anglada, O. Diéguez, J. D. Gale, A. García, J. Junquera, R. M. Martin, P. Ordejón, J. M. Pruneda, D. Sánchez-Portal and J. M. Soler, The SIESTA method; developments and applicability. Journal of Physics: Condensed Matter, 20 (6), 064208, (2008).

[4] J. M. Soler, E. Artacho, J. D. Gale, A. García, J. Junquera, P. Ordejón, D. Sánchez-Portal, Journal of Physics: Condensed Matter, 14 (11), (2002).