Recent and future developments

In siesta™

cecam
Centre Européen de Calcul Atomique et Moléculaire

ICN2
Institut Català de Nanociència i Nanotecnologia

CSIC
Consejo Superior de Investigaciones Científicas

MAX DRIVING THE EXASCALE TRANSITION

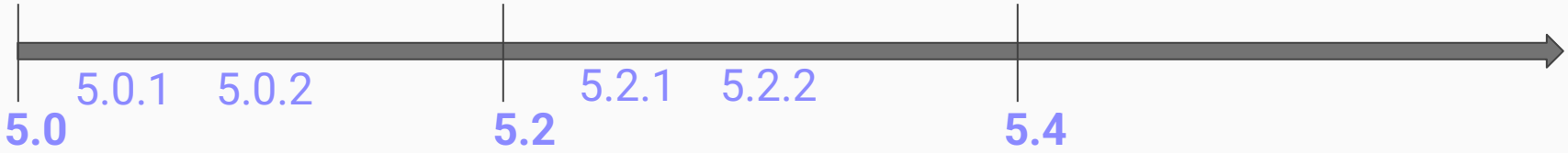
Ministerio de Ciencia, Innovación y Universidades

Financiado por la Unión Europea NextGenerationEU

Plan de Recuperación, Transformación y Resiliencia

Agencia Estatal de Investigación

A timeline



May 2024
PSML, Full SOC, RT-TDDFT, D3, Wannier90 support, updated Basis Set generation, unit and precision standardization

November 2024
Better ELSI integration, improved grid performance, rework of atomic charge output

May 2025

5.4

May 2025

New Feature: QM/MM Calculations

- SIESTA can now do calculations with a field generated by a distribution of point charges.
- More standard QM/MM interface that can be easily leveraged by other MM engines.
- An in-house QM/MM driver is provided.

Performance Improvements

- Added FFTW support for the poisson solver. Optimized distribution in FFT.
- Redesign of the MatEl tables, with a more efficient initialization and additional exploits for better parallel performance.

Utilities

- COOP utilities no longer have internal limitations for inputs, and will default to file extensions like *.bands.WFSX* and *.fullBZ.WFSX* when appropriate.
- Conversion utilities such as vib2xsf, md2xsf, etc. now have improved output formats to allow for larger amount of atoms and better precision overall.
- We now provide a utility to calculate the 2D Lindhard response.

Input/Output

- HSX files have been extended to include cell information, and allow for multiple Hamiltonians in the same file. Also, per-step HSX files can now be written in MD and FC simulations. These updates now **deprecate the TSHS** files for TranSIESTA (so you should stop relying on them).

- **BASIS_ENTHALPY and BASIS_HARRIS_ENTHALPY are also deprecated** in favor of systemlabel.BASIS_ENTHALPY. In addition, a new per-species basis pressure option is provided.

5.4 Features

View the release notes!

https://siesta-project.org/siesta/Documentation/Release_Notes/SIESTA-5.4.0_release_notes.html

HPC tools

Continuously updated

HPC Tools

- Easybuild, SPACK recipes for major EuroHPC clusters:

  https://gitlab.com/siesta-project/ecosystem/build-tools

- SIESTA is also in EESSI!

- JUBE4MaX benchmarking tool for automated benchmarking:

  https://gitlab.com/max-centre/JUBE4MaX

5.6?

September/October 2025

5.6 Expectations

We will be targeting code robustness, small quality of life improvements.

- Code cleanup and better modularization in general, aiming for a more robust SIESTA API.
- Better documentation, extensions and fixes to the build system.
- Extensions to existing features (such as SOC in TS).

5.6 Expectations

Features:

- Parallelization of Vibra and electron-phonon tool (elph).
- SIESTA-ESM.
- Basis Set generation to include non-polarization p orbitals in s-block atoms.
- Hybrids?

5.6 Expectations

Features that might carry over to the next release:

- New integrators/propagators for RT-TDDFT.
- Symmetry support via spglib.
- Implicit solvent support via PSolver.

6.0????

Q2/Q3 - 2026

File formats, precision, input option defaults.