MAX DRIVING THE EXASCALE TRANSITION

siesta

Description

SIESTA is both a method and its open-source computer program implementation, to perform efficient ab initio (DFT-based) electronic structure calculations of molecules and solids. Its accuracy and cost can be tuned in a wide range, from quick exploratory calculations to highly accurate simulations. It incorporates the TranSIESTA transport code.

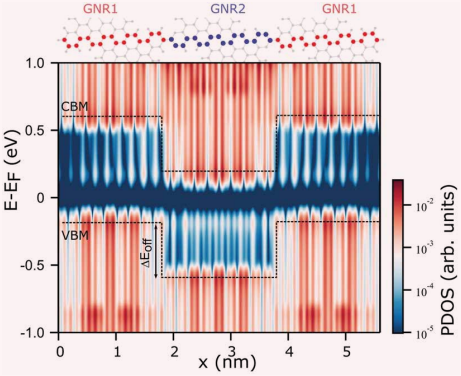
Level of theory

- Density-Functional Theory
- Molecular Dynamics
- Non-Equilibrium Green's Function (NEGF)
- Time-Dependent DFT (TDDFT)
- Quantum Mechanics / Molecular Mechanics (QM/MM)
- DFT+U
- Density Functional Perturbation Theory

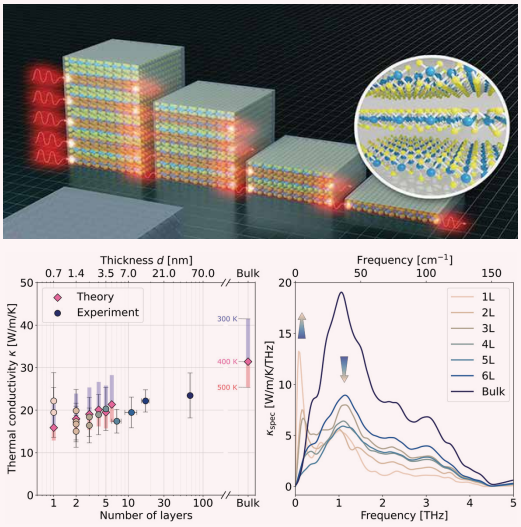
Features

- Design with a focus in algorithmic and computational efficiency.
- Strictly-localised numerical basis sets.
- Now with access to curated pseudopotential databases (in particular Pseudo-Dojo through the PSML format).
- Availability of reduced-scaling DFT methods, down to linear scaling.
- Spin-orbit couplings.
- Range of xc functionals includes van der Waals and hybrid.
- Beyond energies and forces, can compute band structures, densities of states, etc. Rich ecosystem of post-processing tools.
- TranSIESTA transport code (NEGF): open boundary conditions, multiple electrodes, thermo-electric calculations, phonon transport.
- AiiDA-SIESTA plugin for high-throughput computations.

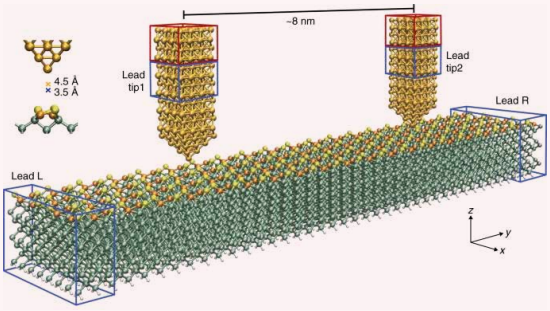
Case studies



Simulated LDOS scan of hybrid nanoporous graphene
[Tenorio et al., Adv. Mater. (2022)]



Heat transport in MoSe2, from bulk to monolayer
[Saleta Reig et al., Adv. Mater. (2022)]



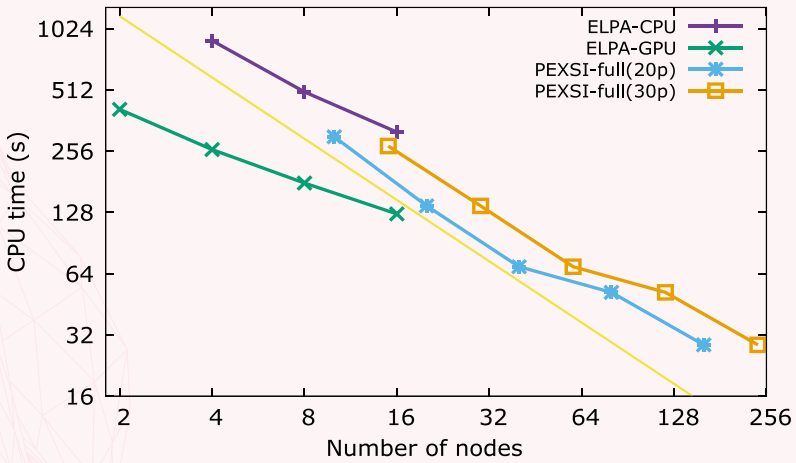
Transport simulations for two-probe STM experiments
[Kolmer et al., Nat. Commun. (2019)]

MAX DRIVING THE EXASCALE TRANSITION

siesta

Parallelization and HPC performance

On top of its algorithmic efficiency, SIESTA is a computationally performant package, written in modern Fortran and with both MPI and OpenMP parallelizations. For most problems, the most computationally-tdemanding stage of SIESTA execution is the solver stage (calculation of energies from the sparse overlap matrix and Hamiltonian). On the one hand, SIESTA provides a range of solvers of its own, from cubic-scaling diagonalisation to linear-scaling methods, that exploit existing linear algebra libraries such as ScaLAPACK, ELPA and DBCSR. On the other hand, SIESTA can leverage a number of libraries that implement favourably-scaling solvers, such as Chess (Fermi Operator Expansion method) and PEXSI (Pole Expansion and Selected Inversion). All these libraries are designed for parallel execution, and they are progressively incorporating support for offloading to an increasing breadth of GPU architectures. SIESTA accesses many of these libraries via their ELectronic Structure Infrastructure (ELSI) interfaces. The figure below exemplifies the scaling of some of these solvers. Note the speed-up provided by GPU offloading, the fact that the (CPU-only) PEXSI solver allows for even shorter times to solution by scaling to a larger number of nodes, and that the increased PEXSI accuracy (30 poles) enables scaling to a larger number of nodes, thus not increasing the time to solution.



Time to solve the diagonalization problem, piece of SARS-COV-2 protein surrounded by water molecules (~58,000 orbitals), Marconi 100 supercomputer (CINECA). Access to ELPA and PEXSI via ELSI.

Support

SIESTA releases (with User's Manuals)

Materials from latest school (2021), including video lectures

Tutorials

Forum

Issue tracker

References

- *J. M. Soler et al., The SIESTA method for ab initio order-N materials simulation, J. Phys.: Condens. Matter* ***14****, 2745 (2002).*
- *N. Papior et al., Improvements on non-equilibrium and transport Green function techniques: The next-generation TRANSIESTA, Comput. Phys. Commun.* ***212****, 8 (2017).*
- *A. García et al., Siesta: Recent developments and applications, J. Chem. Phys.* ***152****, 204108 (2020).*

Acknowledgements

SIESTA is also supported by the Spanish State Research Agency (AEI).

AGENCIA ESTATAL DE INVESTIGACIÓN