siesta
TM

Final remarks

15/11/2024

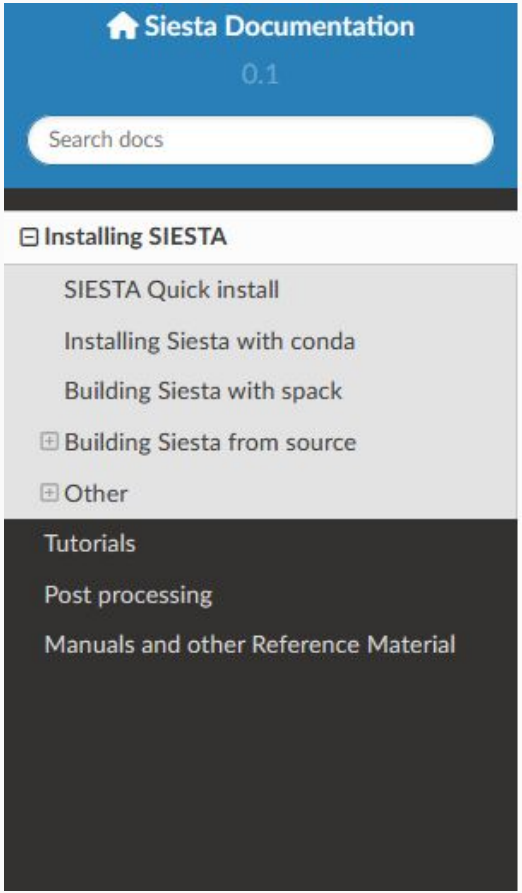
siesta™

Fill the survey!

Your feedback is important!

siesta™

- Spanish Initiative for Electronic Simulations with ***Thousands of Atoms***.
- Works under a few approximations, but enables simulations for very large systems.
- The quality of your calculation is controlled by **you**.
- Lots of different functionalities (MD, NEGF, Phonons, Optical properties, TD-DFT…)
- Under continuous development!



» Installing SIESTA

Installing SIESTA

- SIESTA Quick install
- Installing Siesta with conda
- Building Siesta with spack

Building Siesta from source

- Overview of building SIESTA
- Preparing the environment
- Building Siesta with CMake
- Known issues when building SIESTA

Other

- Installing the FLOS library for Lua

Getting siesta

conda | Building from source | spack

Platforms osx-arm64,osx-64,linux-64

Serial installation:

```
conda install -c conda-forge siesta
```

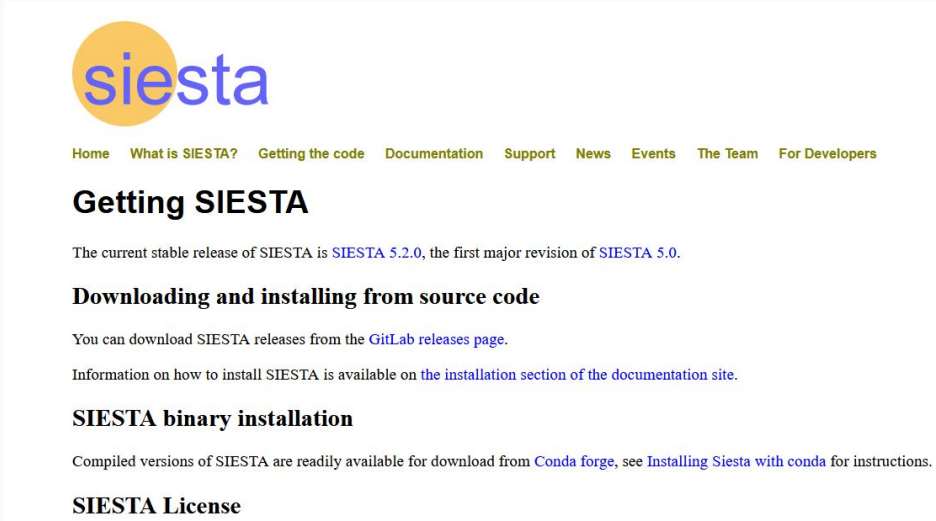
Parallel installation with OpenMPI:

```
conda install -c conda-forge siesta=*=*openmpi*
```

Parallel installation with mpich:

```
conda install -c conda-forge siesta=*=*openmpi*
```

For more details, refer to Installing Siesta with conda.



siesta

Home | What is SIESTA? | Getting the code | Documentation | Support | News | Events | The Team | For Developers

Getting SIESTA

The current stable release of SIESTA is SIESTA 5.2.0, the first major revision of SIESTA 5.0.

Downloading and installing from source code

You can download SIESTA releases from the GitLab releases page.

Information on how to install SIESTA is available on the installation section of the documentation site.

SIESTA binary installation

Compiled versions of SIESTA are readily available for download from Conda forge, see Installing Siesta with conda for instructions.

SIESTA License

Looking back: how do I use SIESTA?

1
Define your problem

Atomic species involved, coordinates (*use databases and programs like avogadro/ase*)

2
Pick a level of theory

Choose DFT functional, look for/generate appropriate pseudopotentials (*read literature!*).

3
Optimize your basis set

Might take from a few hours to a couple of days, depending on system.

4
Converge your mesh and k-point sampling.

Should take only a few minutes to a few hours.

5
GO!

Explore the electronic structure

Plot bands, DOS, look at atomic charges, even get a 3D plot of the density!

Moving atoms

Optimize geometry, run *ab initio* molecular dynamics, or get vibrational modes and phonons.

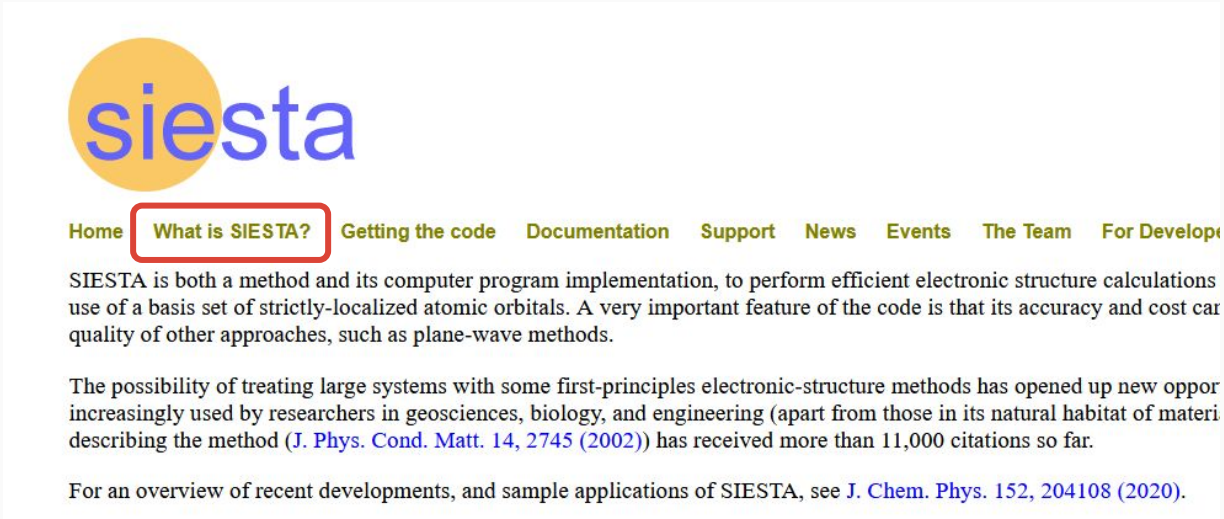
Get more physics out of the electronic density

Get magnetic properties, polarization, apply voltages, and more!

Citing siesta

The SIESTA method for ab initio order-N materials simulation (2002)
DOI: 10.1088/0953-8984/14/11/302

Siesta: Recent developments and applications (2020)
DOI: 10.1063/5.0005077



Where do you go from here?

More tutorials (*pssst: google "siesta docs"*)

https://docs.siesta-project.org/projects/siesta/en/stable/index.html

Basics of Siesta

This section is recommended for all beginners, and also as a refresher for more experienced users.

- A First Encounter - Part 1: Running SIESTA
- A First Encounter - Part 2: Choosing your level of theory
- Basis set optimization
- Basis sets - Tips and tricks
- The real-space grid
- Sampling of the BZ with k-points
- The self-consistent-field cycle
- Analysis tools
- Structural optimization using forces and stresses
- Vibration modes and phonons
- Spins, Magnetism, and Spin-Orbit Coupling
- First crystals

Intermediate and Advanced Topics

This section provides deeper introductions to relevant topics.

- Advanced analysis of the electronic structure
- Molecular Dynamics
- Advanced topics in phonons
- Spin-Orbit coupling
- Polarization calculations with the Berry-phase approach
- DFT+U calculations
- Time-Dependent Density-Functional Theory
- Wannier functions
- Nudged Elastic Band (NEB) Calculations
- Band Unfolding in Siesta
- TranSIESTA

Teach others!

Tutorials exist as stand-alones, and can be followed with little guidance.

Slides from the school are available for you to grab inspiration.

Set of video lectures from 2021:

https://siesta-project.org/siesta/events/SIESTA_School-2021/Lectures.html

Where can you find us?

- SIESTA project web: https://siesta-project.org/siesta/
- Gitlab: https://gitlab.com/siesta-project/siesta
- Discord (same server!)
- Material Stack Exchange: https://mattermodeling.stackexchange.com

Upcoming events

Stay tuned for future events:

- In our webpage:

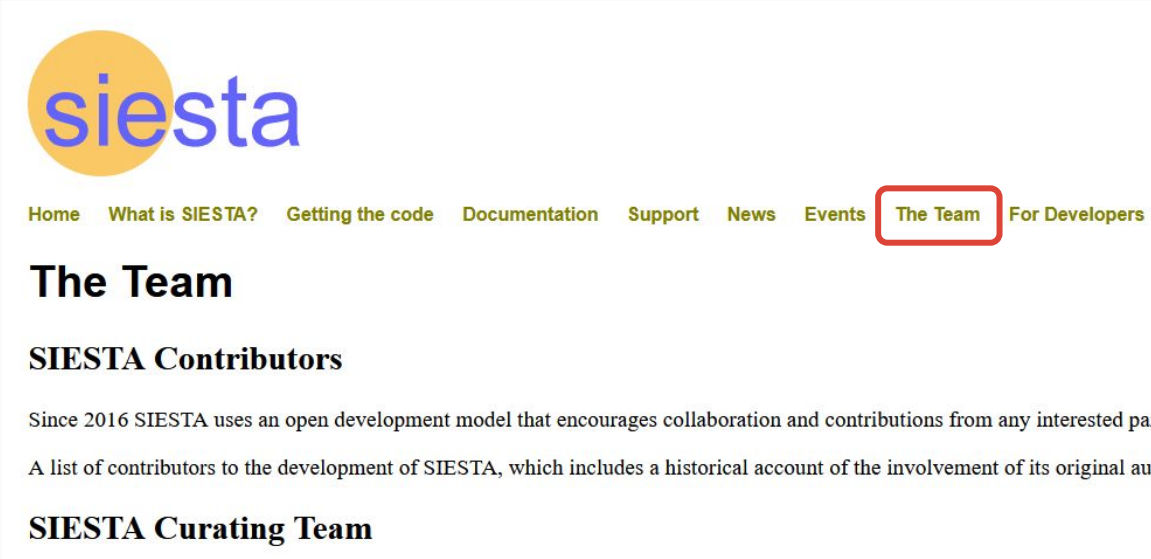
  https://siesta-project.org/siesta/events/

- In our discord server
- Via Psi-K (psi-k.net), MaX (max-centre.eu) and CECAM (cecam.org) newsletters and posts.

Come visit us

SIESTA is done by many people, and there are many groups involved.

Visitors are always welcome!



Special Thanks

Thank you!

All of you students for being here!

Tutors, lecturers and organizers

Sponsors and supporting institutions

See you around!