

siesta Community Guidelines

TM

Interacting with SIESTA beyond the command line



Where is  siesta ?
TM

First, the webpage:

<https://siesta-project.org/siesta/>



What is SIESTA?

Getting the code

Documentation

Support

News

Events

The Team

For Developers



GOBIERNO
DE ESPAÑA

MINISTERIO
DE CIENCIA, INNOVACIÓN
Y UNIVERSIDADES



- **Links to every other page that is SIESTA related.**
- Information on events organized by us and other SIESTA groups.
- Contact information.
- Info on basic gitlab interactions for starting developers.

Tutorials and documentation:

<https://docs.siesta-project.org/projects/siesta/en/stable/>



The screenshot shows the Siesta project website. At the top is the 'siesta' logo, consisting of an orange circle and the word 'siesta' in blue. Below the logo is a row of statistics: 'Original paper 14511', 'Latest paper 428', 'Original TranSIESTA paper 6166', and 'Latest TranSIESTA paper 403'. Below this is another row: 'conda | conda-forge v5.2.2' and 'downloads 256k total'. The main text states: 'SIESTA is a program for efficient electronic structure calculations and ab initio molecular dynamics simulations of molecules and solids in the framework of Density-Functional Theory (DFT)'. There are four buttons with icons: a wrench for 'Installation', a person for 'Tutorials', a book for 'User guide', and a speech bubble for 'Chat with us'. Each button has a short description. At the bottom right is a 'Next' button with a right arrow.

Original paper 14511 Latest paper 428 Original TranSIESTA paper 6166 Latest TranSIESTA paper 403

conda | conda-forge v5.2.2 downloads 256k total

SIESTA is a program for **efficient electronic structure calculations** and ab initio molecular dynamics simulations of molecules and solids in the framework of **Density-Functional Theory (DFT)**.

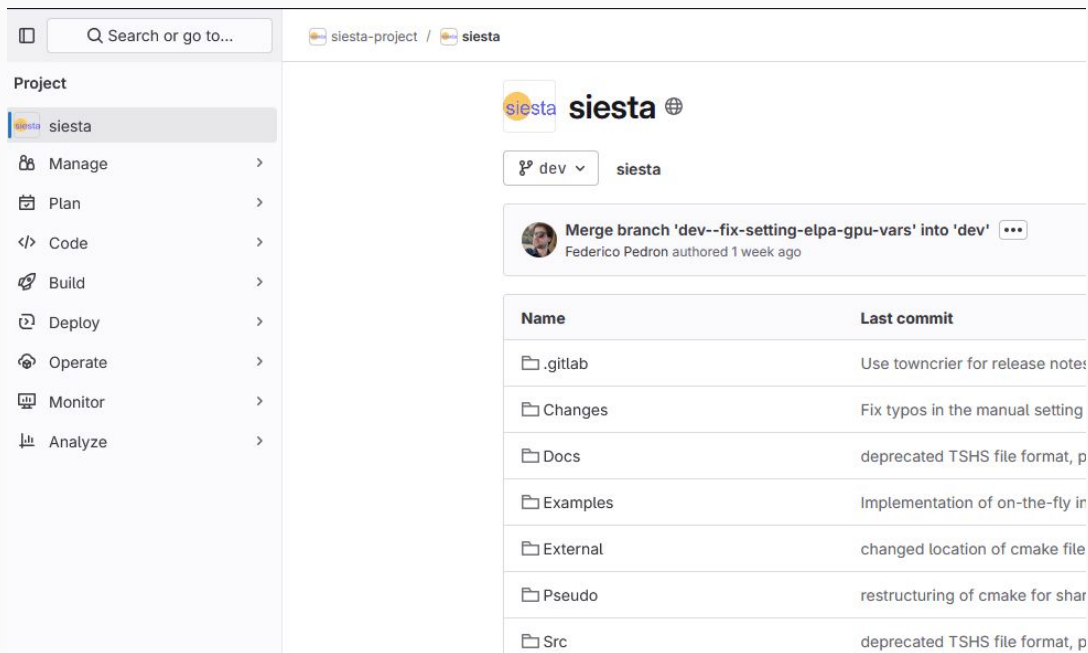
- Installation.
Installing SIESTA is easier than you might think, check out our quick installation guide.
- Tutorials
Let us show you how to do things with SIESTA!
- User guide
Explore all the features of SIESTA.
- Chat with us
Join our Discord channel to share results or get help.

Next →

- Tutorials are in constant improvement.
- There is an online version of the manual!

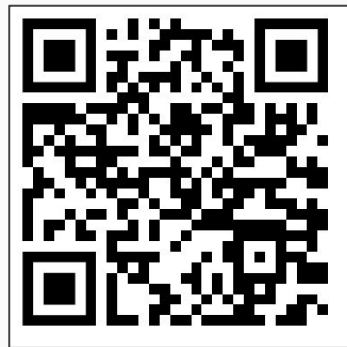
GitLab

<https://gitlab.com/siesta-project/siesta>



The screenshot shows the GitLab web interface for the `siesta-project / siesta` repository. On the left is a sidebar with navigation links: Project, Manage, Plan, Code, Build, Deploy, Operate, Monitor, and Analyze. The main content area displays the repository name `siesta` with a globe icon, a dropdown menu set to `dev`, and a recent commit by Federico Pedron titled "Merge branch 'dev--fix-setting-elpa-gpu-vars' into 'dev'". Below this is a table listing the repository's structure.

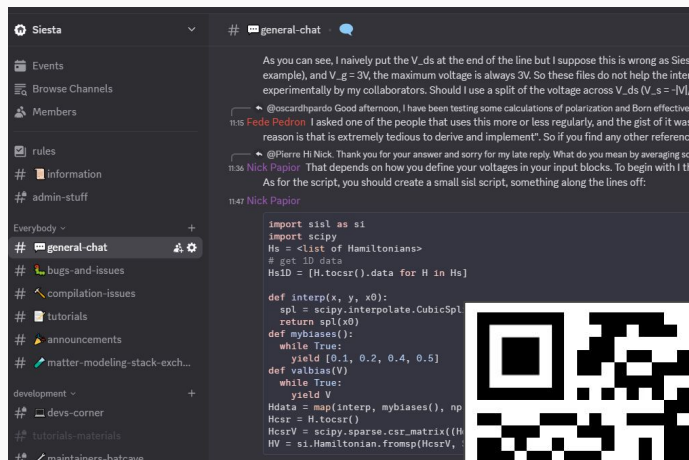
Name	Last commit
<code>.gitlab</code>	Use towncrier for release notes
<code>Changes</code>	Fix typos in the manual setting
<code>Docs</code>	deprecated TSHS file format, p
<code>Examples</code>	Implementation of on-the-fly in
<code>External</code>	changed location of cmake file
<code>Pseudo</code>	restructuring of cmake for shar
<code>Src</code>	deprecated TSHS file format, p



- Bug reports
- Code development

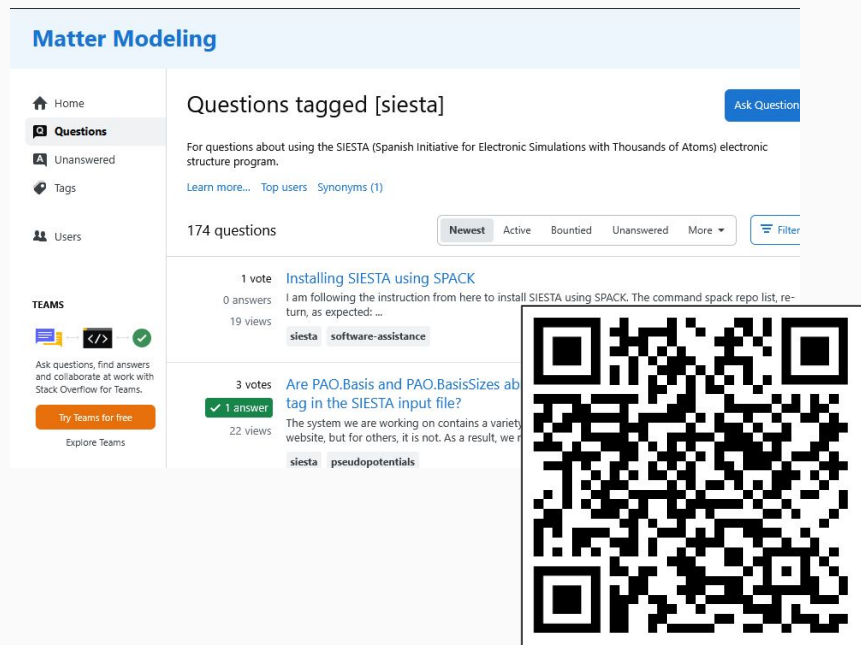
Discord

<https://discord.gg/AqjX6aTNXR>



Matter Modelling Stack Exchange

<https://mattermodeling.stackexchange.com>



Questions, bug reports, feature requests

Asking questions

Questions on general physics, discussions, literature:

- Ask them on Matter Modeling Stack Exchange! Replies will not be fast, but they're often thorough. Also, people from other codes also collaborate there.

Small questions on SIESTA usage, bugs or installation issues:

- Go to the discord! We usually reply fast, and do not leave questions out.

Asking questions

Please use **gitlab** for feature requests, thorough bug reports, or performance reports.

You can also do it via discord or email, but creating an issue in SIESTA's gitlab is the cleanest way (and saves us a lot of work). So if you're able, please do it!

Submitting code

To interact with SIESTA at the software development level, **gitlab usage is mandatory**:

- we expect you to at least have a minimal knowledge on how git and gitlab works (**and if you don't, ask!** We're always ready to help).
- This is so we can keep proper records of who added which modification to the code.



Code submission

If you're working on a new development for SIESTA, please open an issue and/or MR in the main repo: *this way we get to know who is working on what.*

If your addition to SIESTA is large or complex (or very disrupting) please coordinate with maintainers before rushing headlong into an implementation.

As soon as you want to, *open a merge request* towards the main repo with your developments.

For the code to be merged, we actually require few things:

- The code must be tested enough. The tests within SIESTA at least should work properly. If there's a new functionality, a new test for that functionality is also expected.
- The code must be well documented, and comply with a given coding style. People should not rely on the original developer to explain the code.
- A release notes file should be added under /Changes (see the readme at /Changes/README.md).
- Any new fdf options or run modes should be documented in the manual (under /Docs) in LaTeX format.

Opening a Merge Request is **the first step**, it **does not mean your work is done!**

We might ask for:

- Specific tests for compatibility.
- Added documentation
- Consistency with other SIESTA internals or existing input options (if we already have *NumberOfAtoms*, avoid doing your own *TotalAtoms* input option).

Code submission










Are you bored, have some free time,
and want to collaborate?

Check out the “needs-collaborator”
milestone; it usually has features that
we have been leaving out due to time.

<https://gitlab.com/siesta-project/siesta/-/milestones/15#tab-issues>



Project

-  siesta
-  Manage >
-  Plan v
- Issues
- Issue boards
- Milestones**
- Iterations
- Wiki
- Requirements
-  Code >
-  Build >
-  Deploy >
-  Operate >
-  Monitor >
-  Analyze >

needs-collaborator

This includes stuff that might be useful but we need extra ha

Issues 22 Merge requests 0 Participants 4 L

Unstarted Issues (open and unassigned) 14 0

Extend DM.InitSpin functionality

#476 **feature**

Constraining lattice vectors and angles

#428 **feature**

Electron Localisation Function

#374 **feature**

Read in EDM from file

#276 **feature**

Revisit madelung.f for energy corrections in charged molecule/atom calculations

#241 **feature**

Allow per-species use of 'user-basis'

#234 **feature**

Compatibility of WFS2LDOS (ol-stm) and WsXM

#124 **feature**

STS spectra at given points

#113 **feature**

Computing KS orbitals and saving them to a portable format

#101 **feature**