MAX DRIVING THE EXASCALE TRANSITION

siesta™

SIMUNE ATOMISTICS

User support in the SIESTA ecosystem

Mónica García Mota (Simune Atomistics SL)

ascale", has received funding from the European Union's Horizon 2020 project call H2020-INFRAEDI-
8

USER SUPPORT IN THE SIESTA ECOSYSTEM

USER SUPPORT

MAX DRIVING THE EXASCALE TRANSITION

siesta™ COMMUNITY

SIMUNE ATOMISTICS

Technical support for SIESTA

MaX USERS' SUPPORT SERVICES

- Support for MaX codes and beyond (supporting also some other codes in material science area)
- **High level consultancy**: support end-users and communities by direct consulting and ad-hoc solutions, possibly comprising codes development and refactoring

http://www.max-centre.eu/services

Examples of MaX support actions

- Investigation of **the possible causes of a job failure and solution** of the related problems
- Evaluation of the **MaX codes performance on different architectures**
- Analysis of MaX codes anomalies wrt documentation (e.g. non-converging algorithms)
- **Debugging of problems due to a specific code implementation** (e.g. GPU, MPI, OpenMP versions)
- Selection of the best code parameters that minimize the time to achieve a converged solution
- Optimization of the computational setup to **maximize the performance of a certain simulation on a given architecture** (e.g. find the best combination of number of nodes, number of cores, number of mpi processes/threads, etc...)
- Support in the usage of different **releases of MaX codes** (user guidance about new vs deprecated features)

MaX USERS' SUPPORT SERVICES

Support offered in **two different ways**:

- **by each code community via forum/mailing lists**, where the responsible is always a specialist acting on behalf of MaX;

  siesta™ https://departments.icmab.es/leem/SIESTA_MATERIAL/Docs/list.html

- **via the MaX Help-desk operated by Cineca**

  for each request a ticket is opened in a queue dedicated to MaX.

  HELP DESK support@max-centre.eu

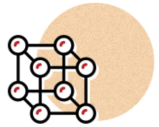
SIMUNE & SIESTA-PRO PROJECT

SIMUNE ATOMISTICS

SIMUNE was launched in 2014 as a joint venture of developers of SIESTA* and ANT**codes, and Nanoscience Cooperative Research Center CIC nanoGUNE.

* Pablo Ordejon, Emilio Artacho and Jose Soler
**Juan José Palacios

SERVICES:



Material Design

Code Support Progam

SIESTA Support

PRODUCT:

ASAP

ATOMISTIC SIMULATION ADVANCED PLATFORM

SIMUNE & SIESTA-PRO PROJECT

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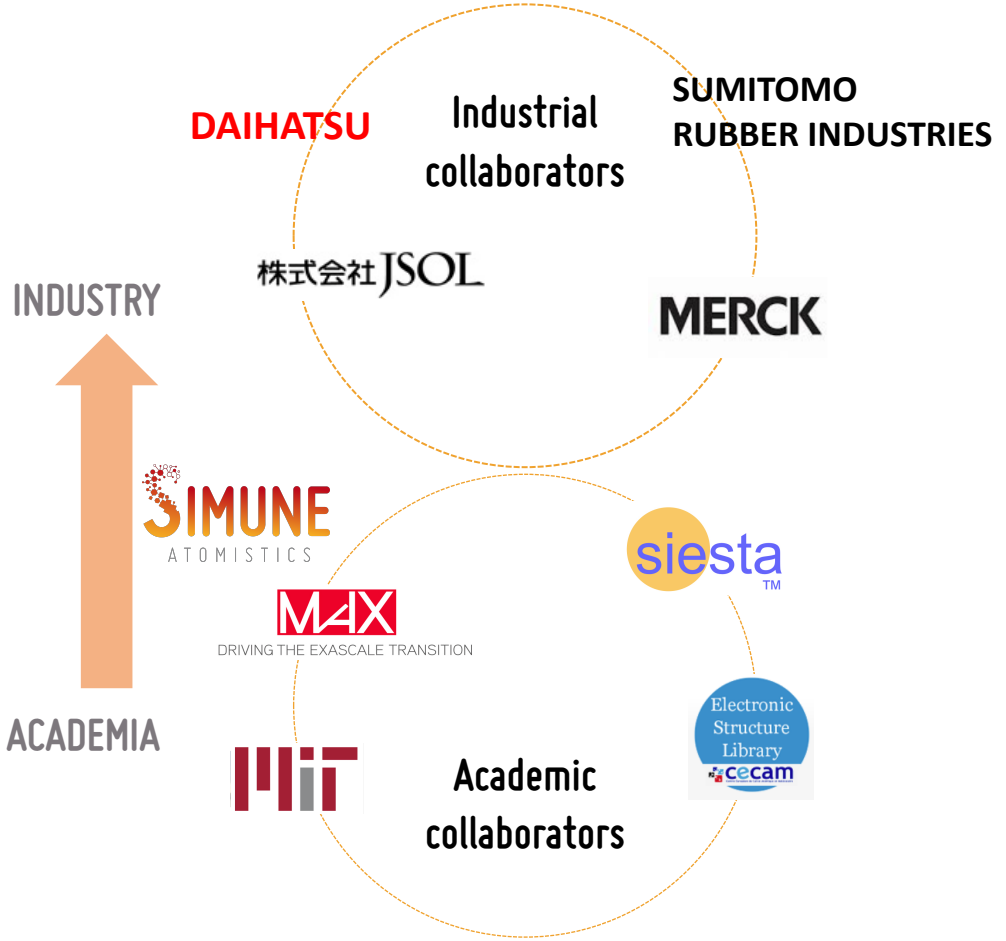

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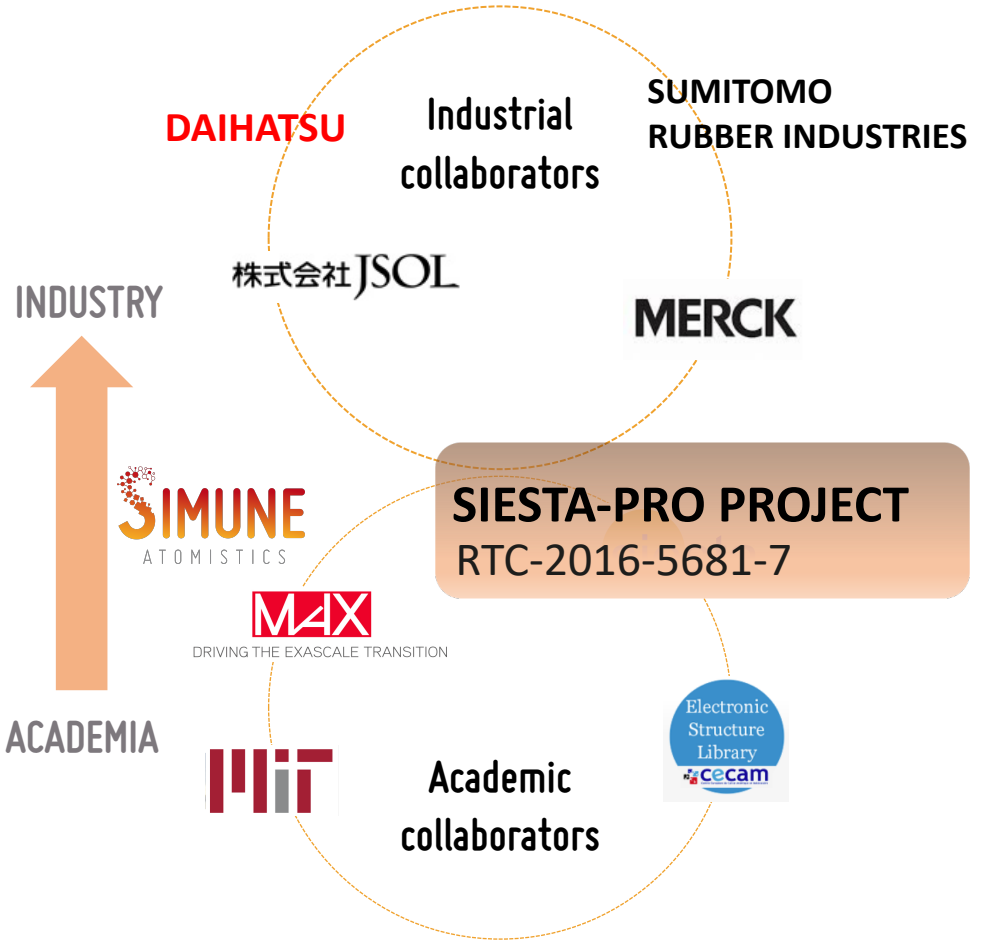
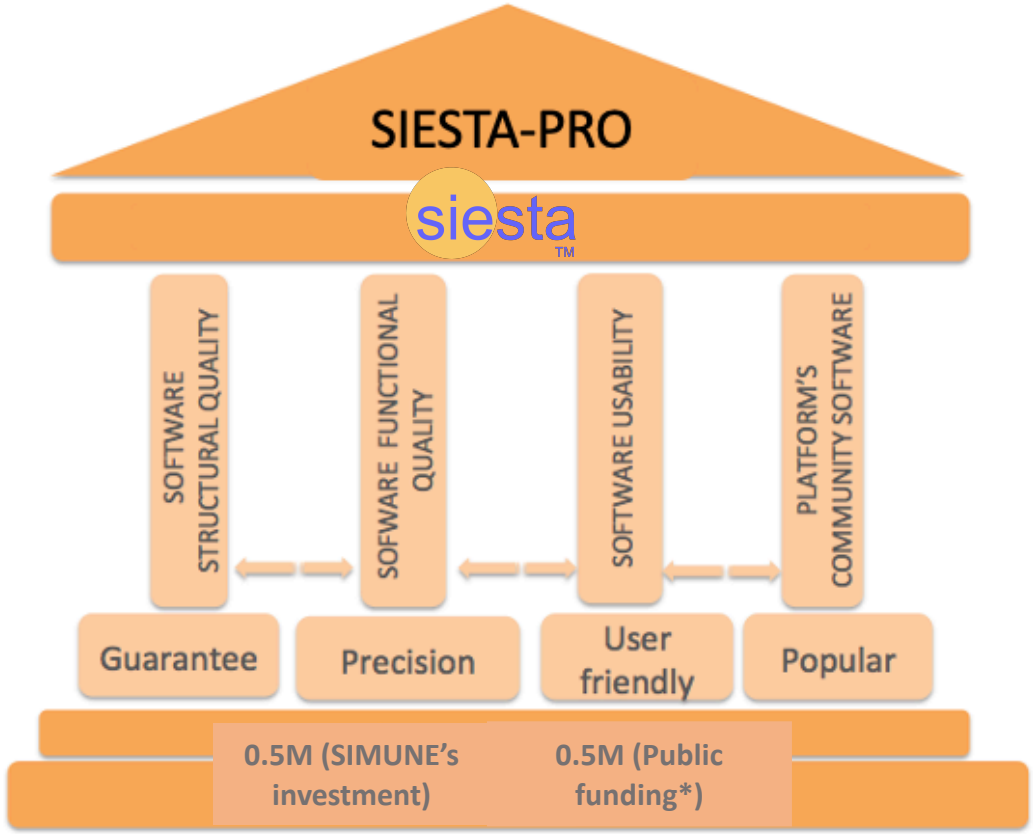


SIESTA-PRO PROJECT

SIESTA-PRO – Spanish Initiative for Electronic Simulations with Thousands of Atoms: Open Source code with professional support and warranty
(2016-2020)

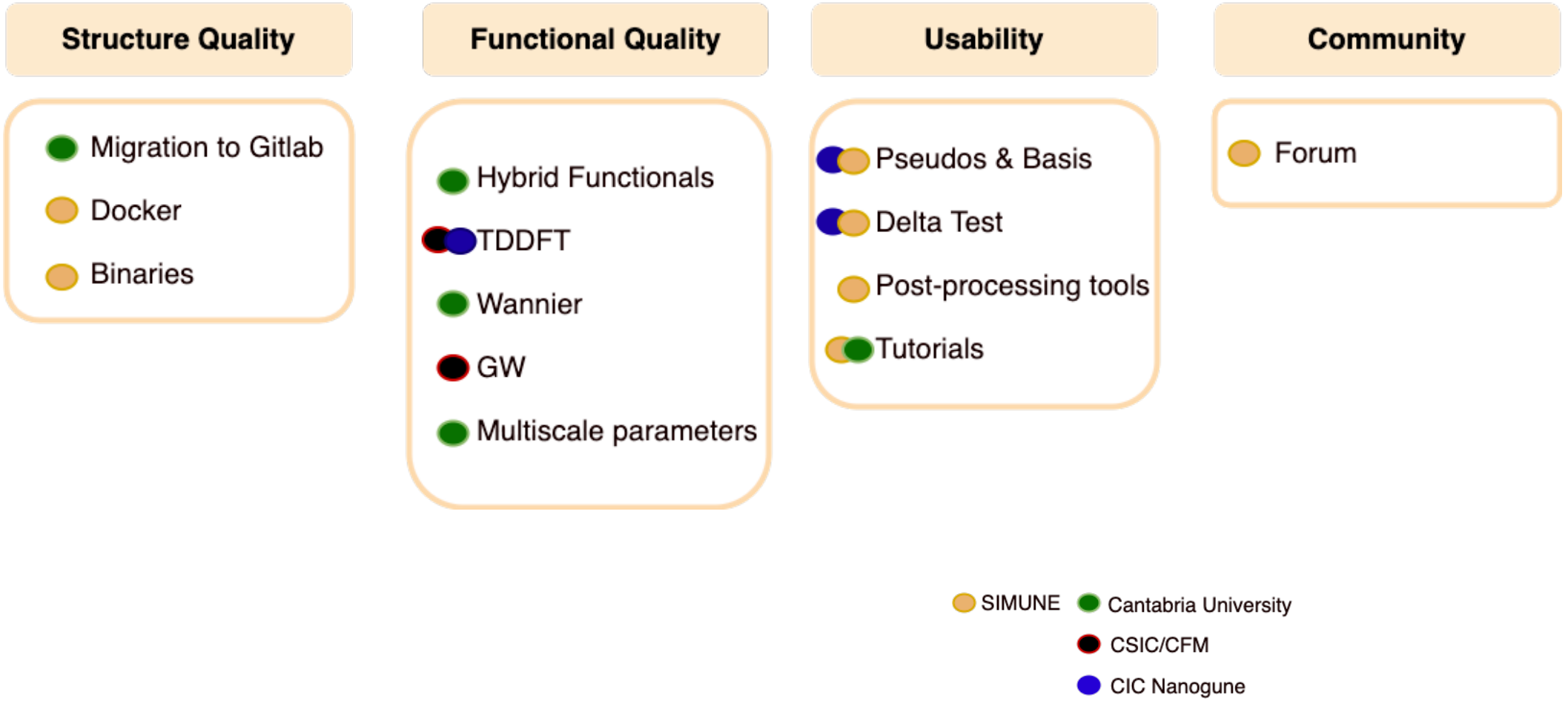
<u>Project partners:</u>
SIMUNE (project coordinator)
UC: Y. Pouillon & J. Junquera
CSIC-CFM: P. Tarifa & D. Sanchez-Portal
CIC NanoGune: D. Lopez & E. Artacho



*The project (RTC-2016-5681-7) has been funded by the Spanish Ministry of Economy, Industry and Competitiveness and has been co-financed by the European Structural and Investment Funds with the objective to promote technological development, innovation and quality research.

SIESTA-PRO PROJECT

Deliverables:



SIESTA-PRO PROJECT

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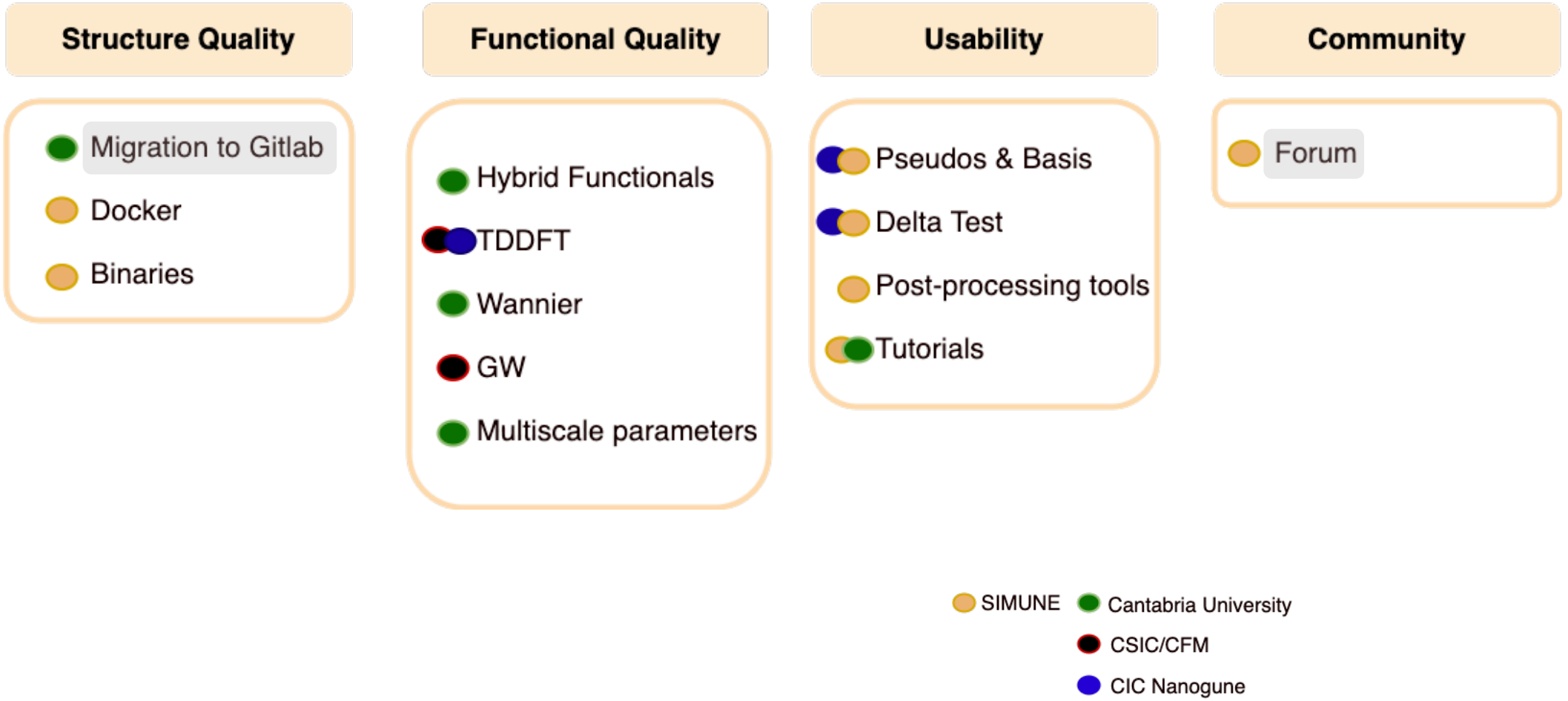
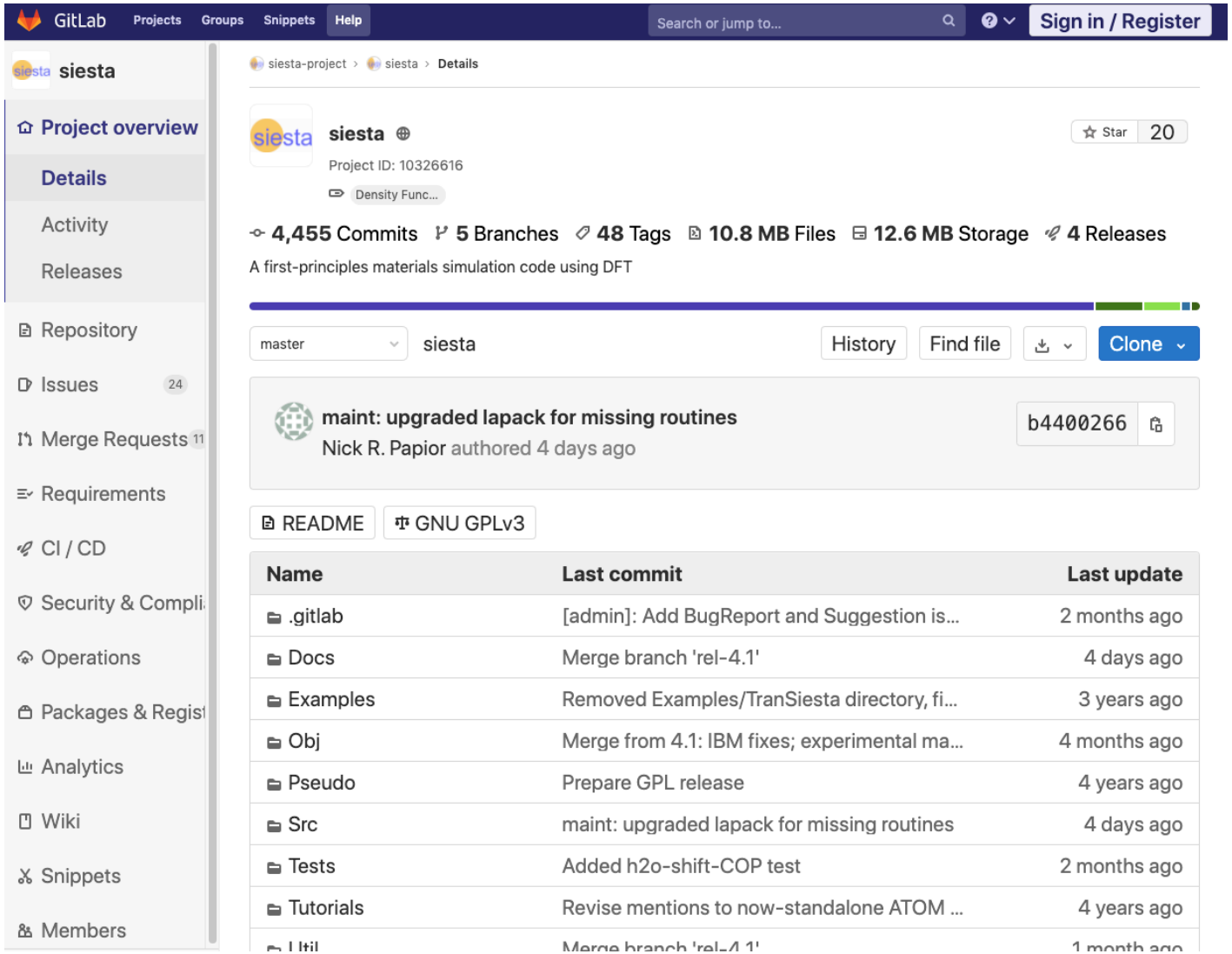


SIESTA COMMUNITY

Migration to Gitlab:



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

SIESTA COMMUNITY

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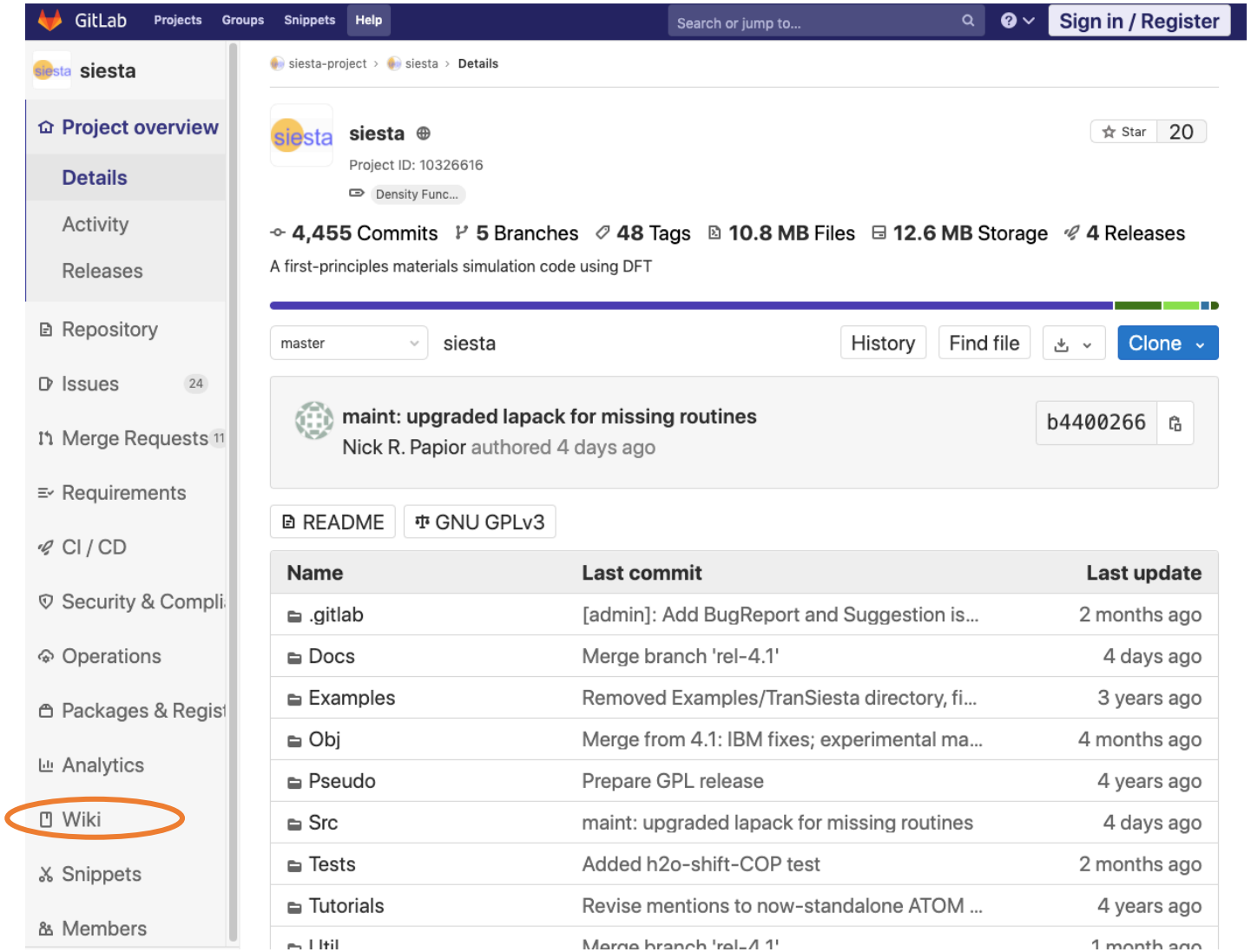

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SIESTA COMMUNITY

Wiki

User documentation

- Overview of user documentation ← SIESTA manual & tutorials
- Guide to Siesta versions ← Information on stable, beta-release & development branches

Developer documentation

- Getting Started with Git and Gitlab
- Contributing to SIESTA
- Migration from Launchpad to Gitlab

https://gitlab.com/siesta-project/siesta/-/wikis/home

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Other Relevant Topics ←

building Siesta
running with GPUs
using PSML pseudopotentials
using Lua

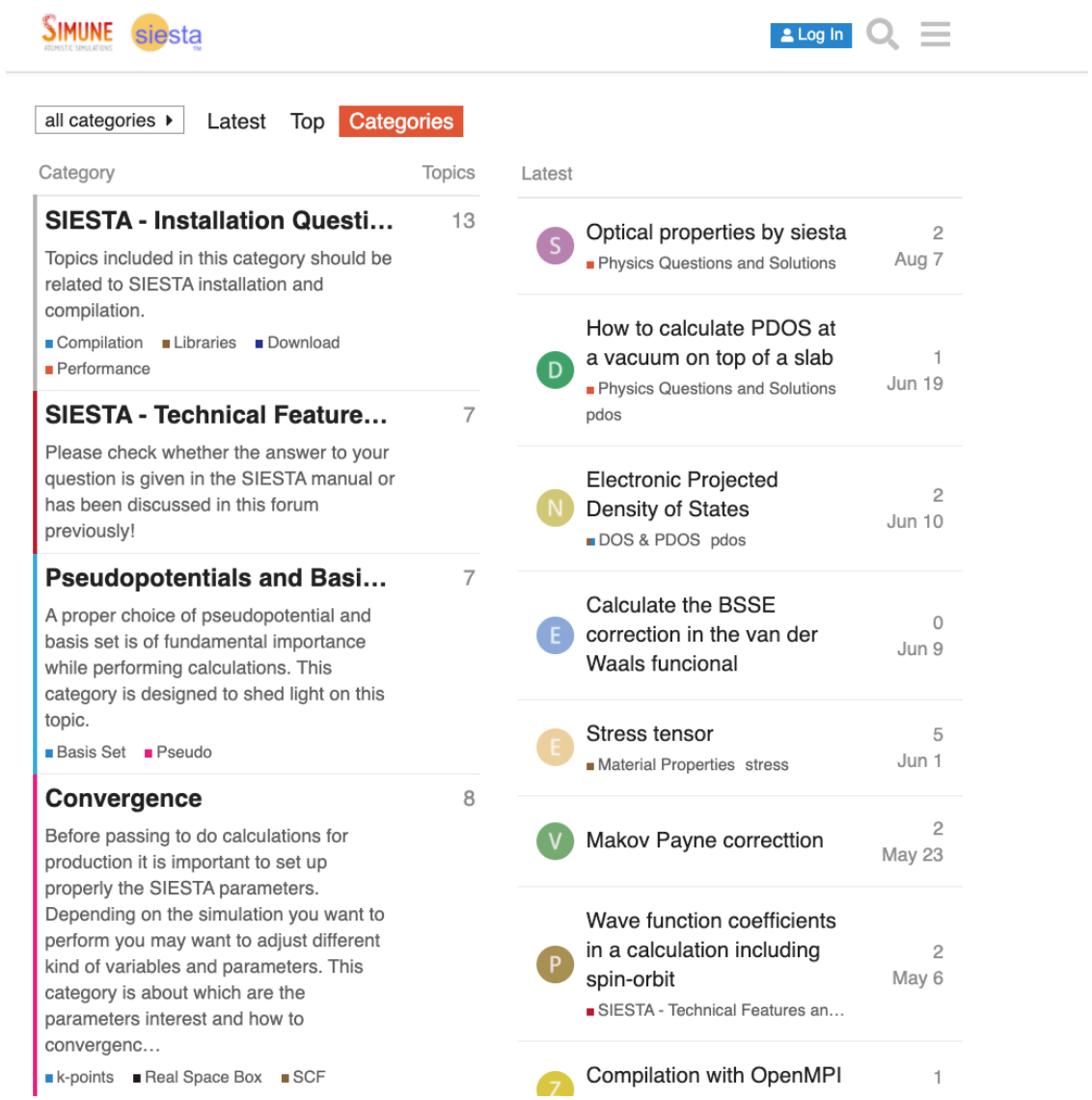
https://gitlab.com/siesta-project/siesta/-/wikis/home

SIESTA COMMUNITY

Forum:

- Summarizes the most relevant Q&A from SIESTA Mailing List
https://departments.icmab.es/leem/SIESTA_MATERIAL/Docs/list.html

- Topics are classified in Categories



https://forum.simuneatomistics.com/

SIMUNE ACTIVITIES

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SIMUNE ACTIVITIES

Automatization/Installation Tools:

- Binaries
  - Compilation/generation of SIESTA binary for Unix system (MacOS, any Linux distribution including HPC architectures)
  - Compilation/generation of SIESTA binary for Windows 10
- Docker
  - Deployment of SIESTA **Docker** images

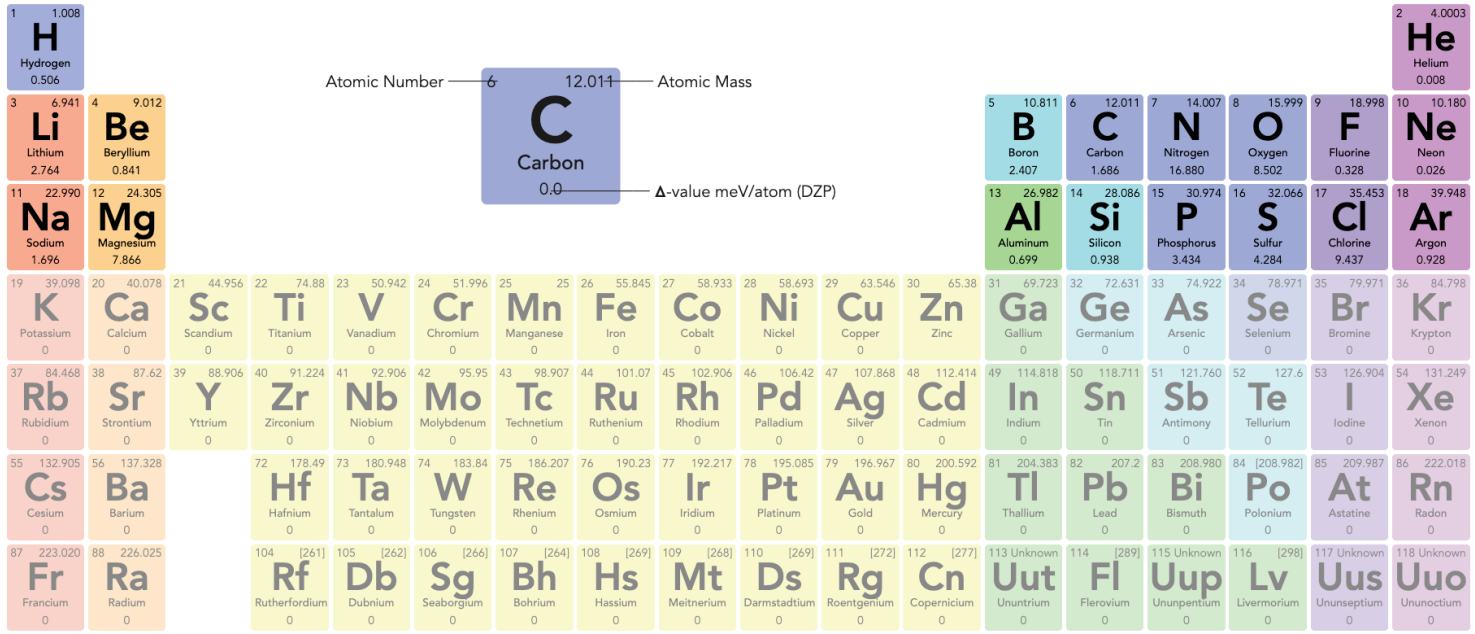

Accessible from: https://www.simuneatomistics.com/downloads/

@ Request SIESTA Binary for Windows

@ Request SIESTA Docker

SIMUNE ACTIVITIES

Pseudopotential (psf) & Basis Sets:



Accessible from:
https://www.simuneatomistics.com/downloads/

For PSML Pseudopotentials: http://www.pseudo-dojo.org/

SIMUNE ACTIVITIES

Graphical User Interface:

- Integration of open-source codes
- User-friendly
- Customer support
- Multiplatform

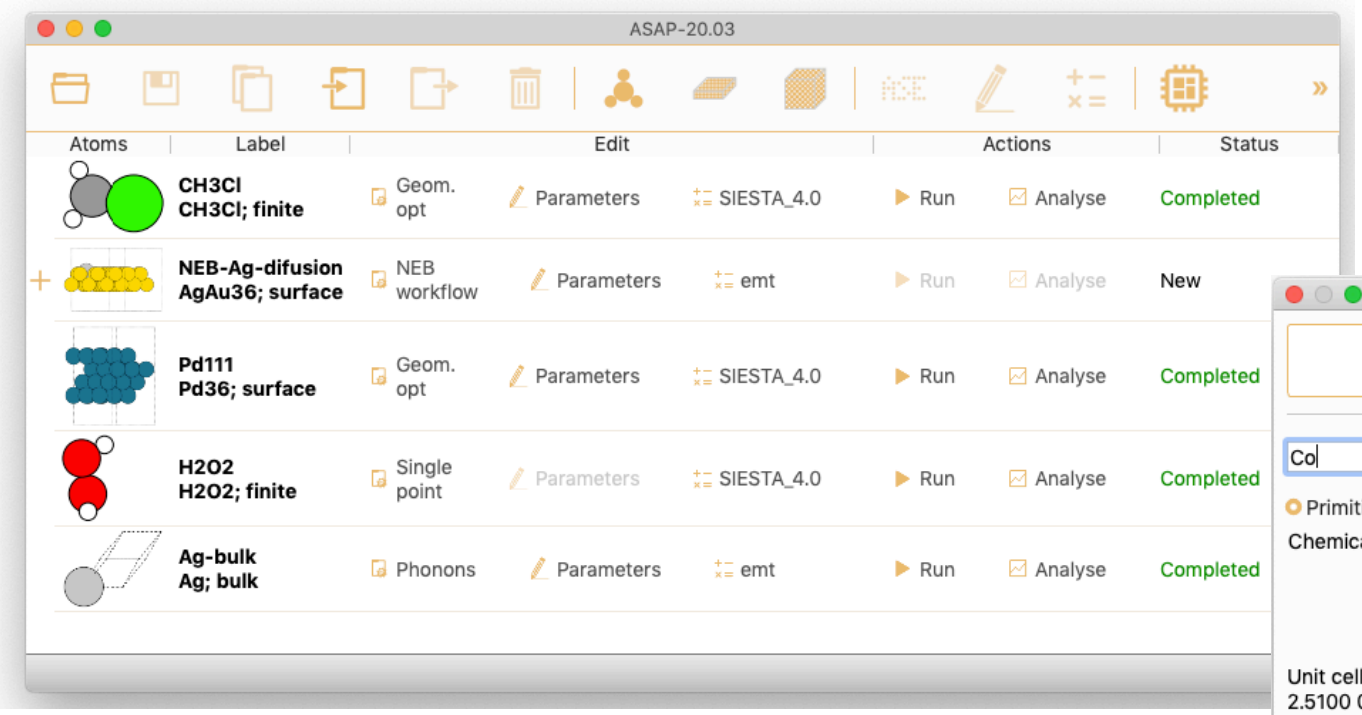
REQUEST ASAP TRIAL VERSION

https://www.simuneatomistics.com/services-products/asap-software/

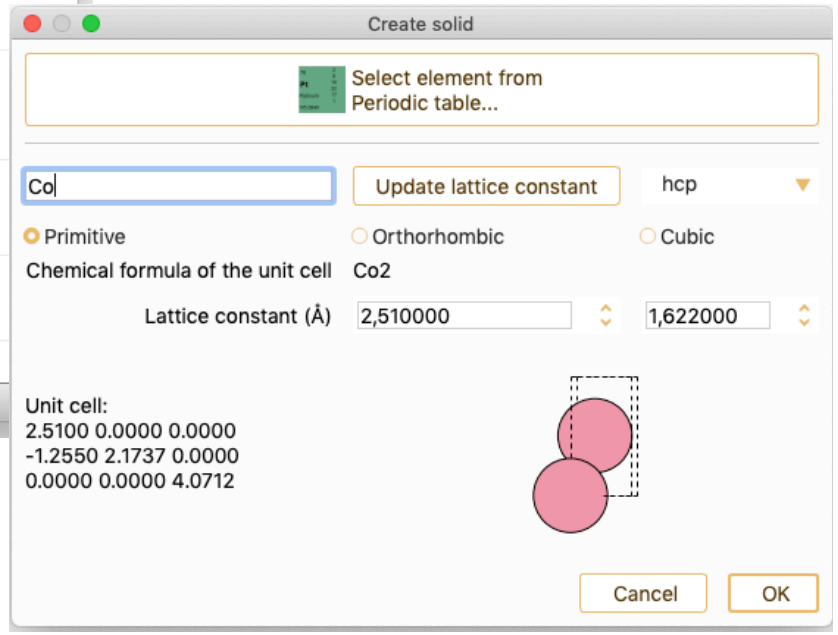
ASAP 20.03 Next Release: 20.10
ASAP developers: J. Alberdi, J. Albizuri, P. Koval, A. Larsen, F. Marchesin Y. Pouillon

SIMUNE ACTIVITIES

ASAP Main Window



The Atomic Structure Builder



SIMUNE ACTIVITIES

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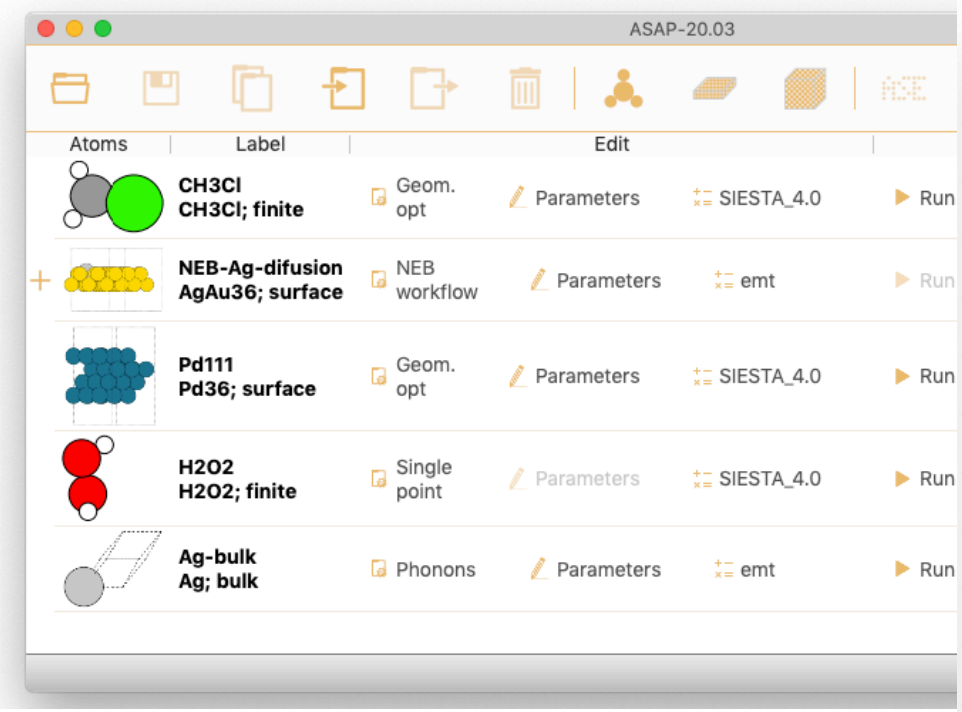
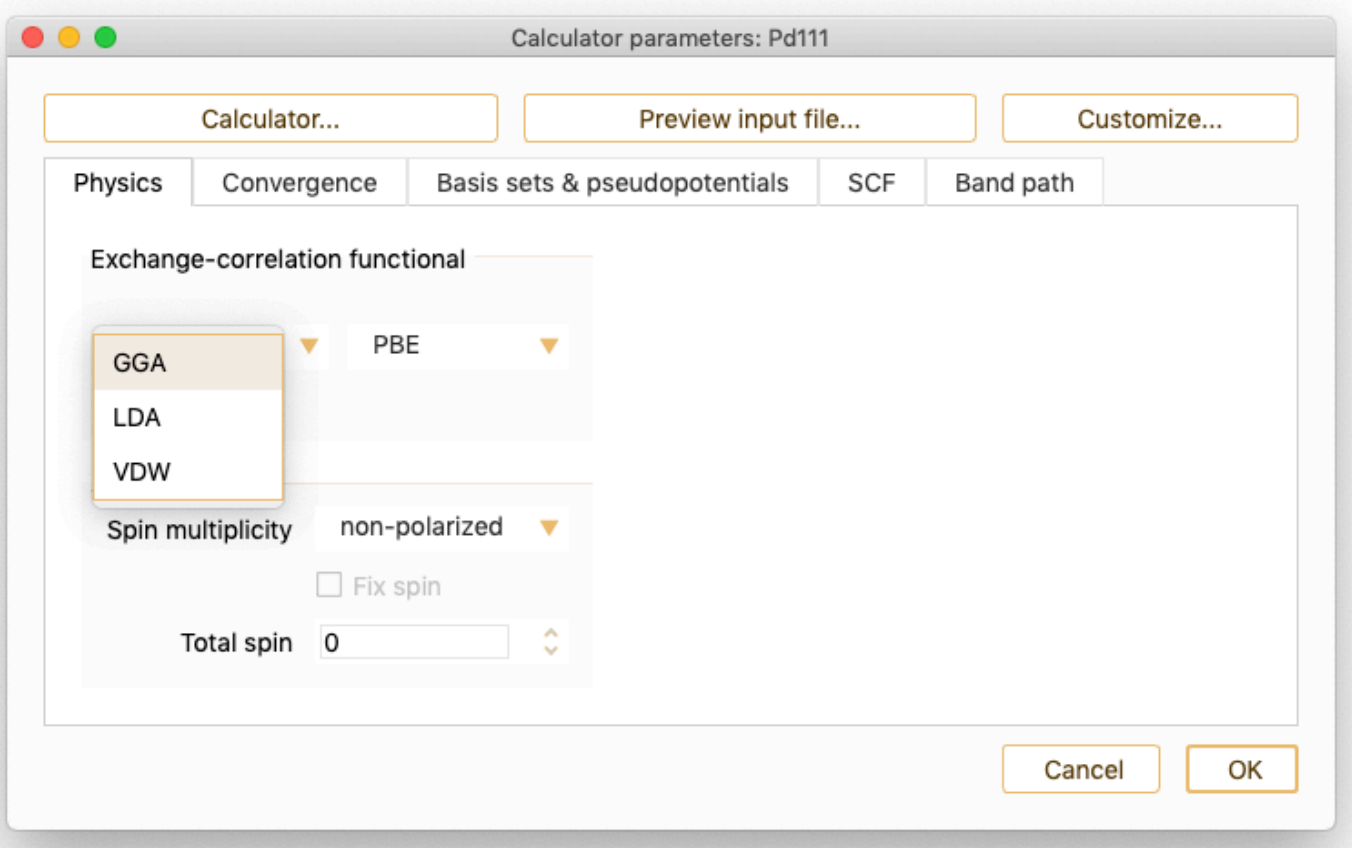


The SIESTA Calculator



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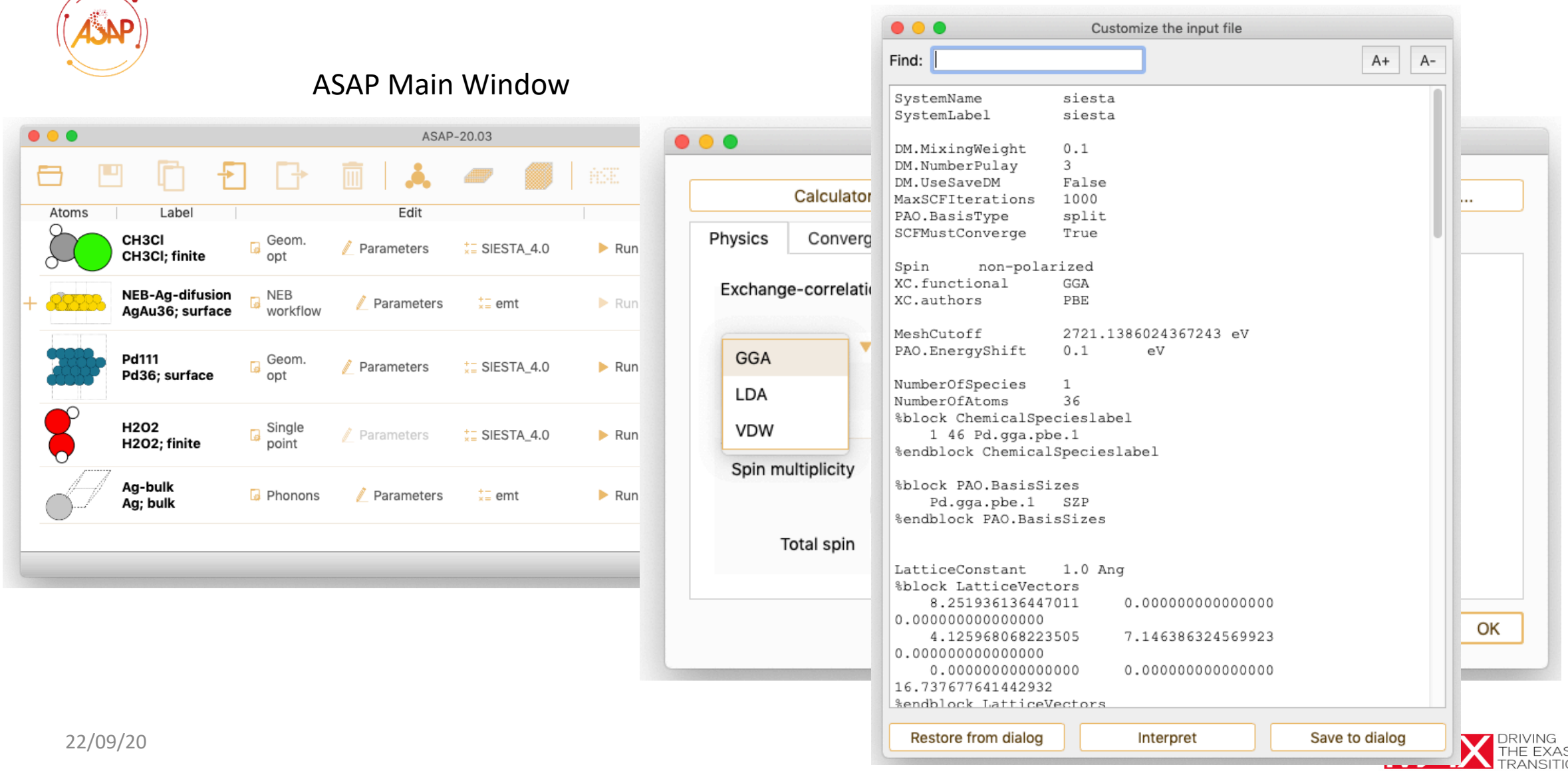

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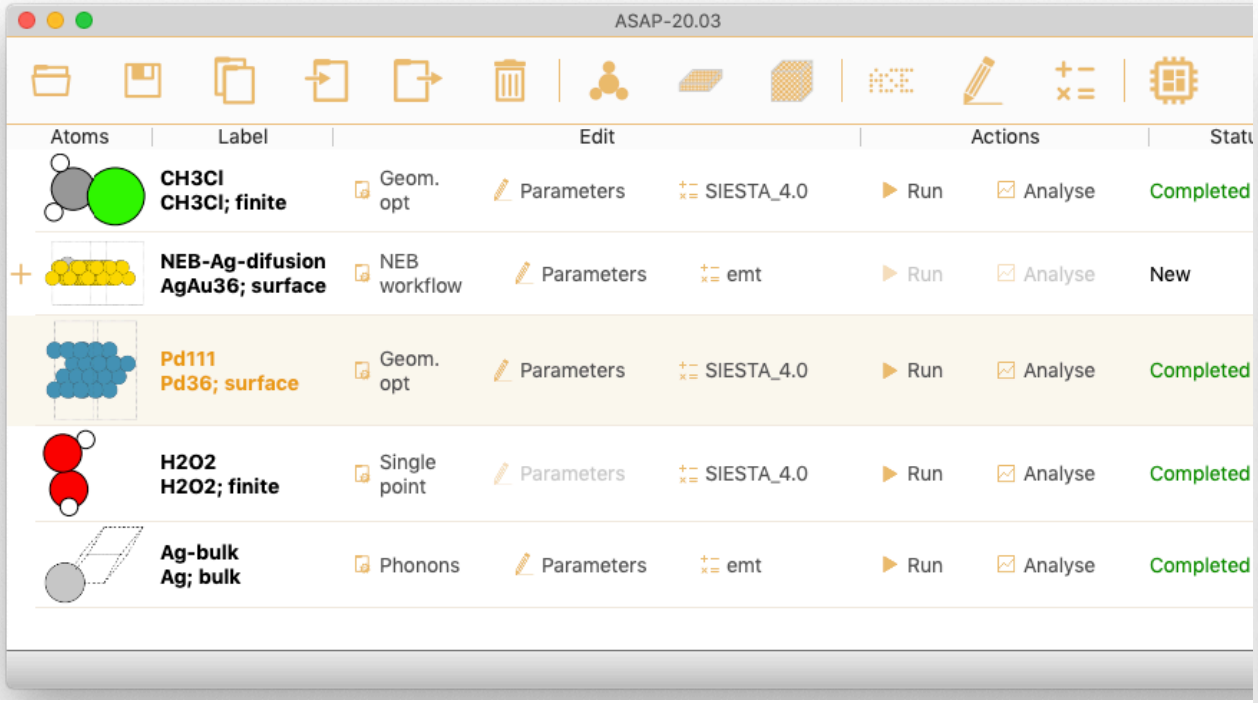
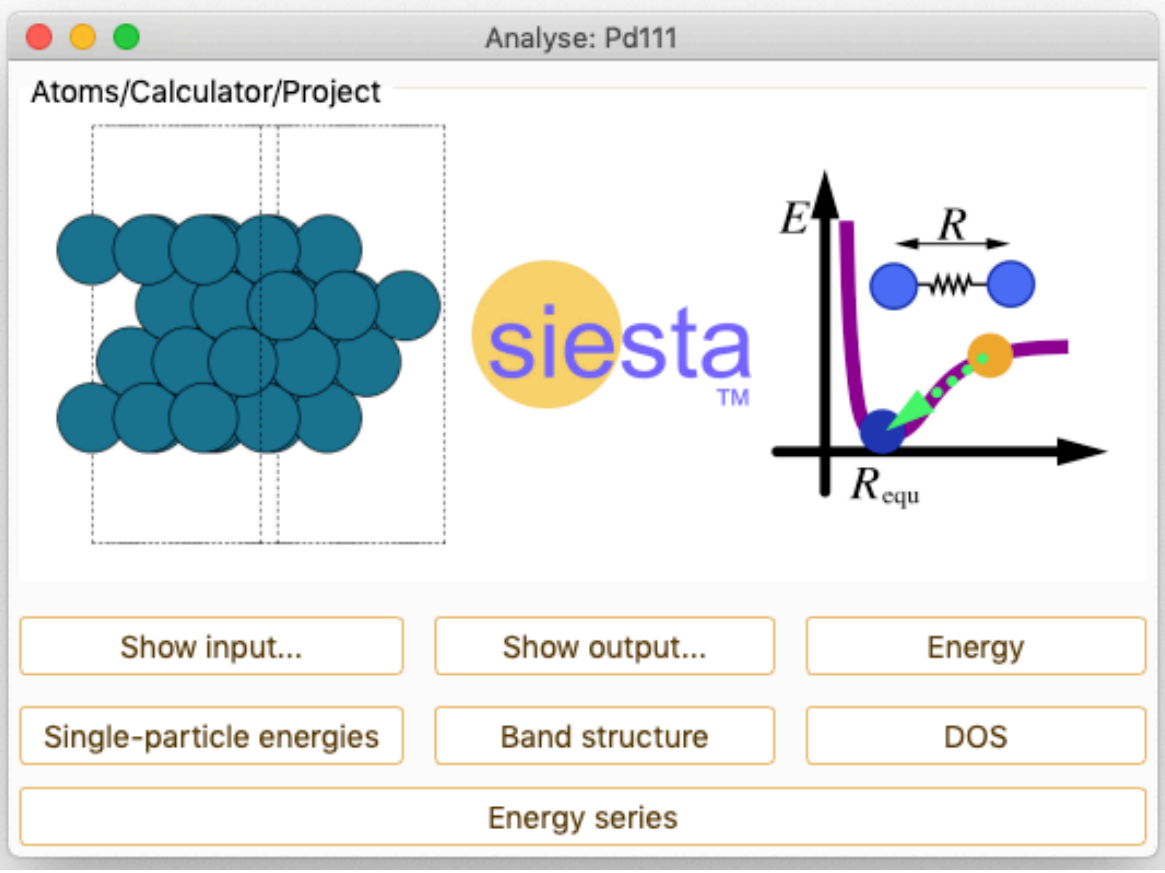


Analysis Widget



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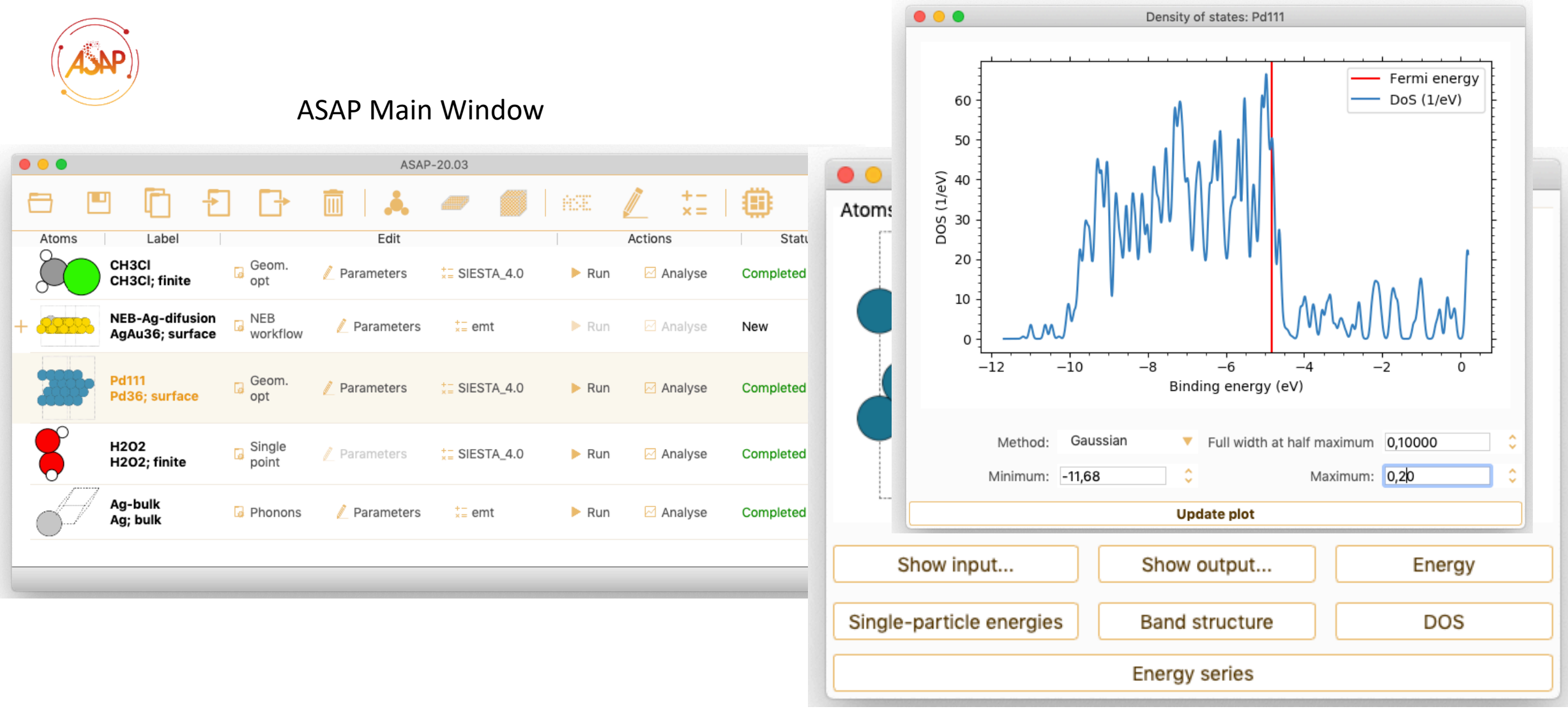

DRIVING THE EXASCALE TRANSITION

THANKS

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company/max-centre/

@max_center2

http://www.max-centre.eu/