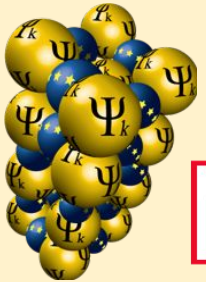
siesta™ Advanced Workshop

Psi-k and CECAM Flagship Workshop
Barcelona, 2-5 June 2025



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

Welcome!

Catalina

Roberta

Federico

José María

Miguel

Day 1: 02/06/2025	Chair: Dr. Federico Pedron	14:00 to 14:30 - Registration
		14:30 to 15:00 - Welcome & Introduction. Dr. Federico Pedron
		15:00 to 17:00 - Electrochemical properties using TranSIESTA and QM/MM - Speakers: Dr. Emane de Freitas Martins | Dr. Pol Febrer
		17:00 to 17:30 - Coffee break
		17:30 to 18:30 - Showcase: Electronic transport - Speaker: Prof. Aran Garcia-Lekue
Day 2: 03/06/2025	Chair: Dr. Miguel Pruneda	**09:00 to 10:30 - Postprocessing using sisl and external control of SIESTA through LUA. Speaker: Dr. Nick Papior**
		10:30 to 11:00 - Coffee break
		11:00 to 13:00 - Magnetism: from SOC to TB2J and beyond. - Speaker: Dr. He Xu
		13:00 to 14:00 - Lunch
		14:00 to 15:30 - Superconductivity - Speaker: Arnold Kole
		15:30 to 16:00 - Coffee break
		16:00 to 17:00 - Showcase: DMFT - Speaker: Prof. Aldo Romero
		20:30 to 22:30 - Social dinner

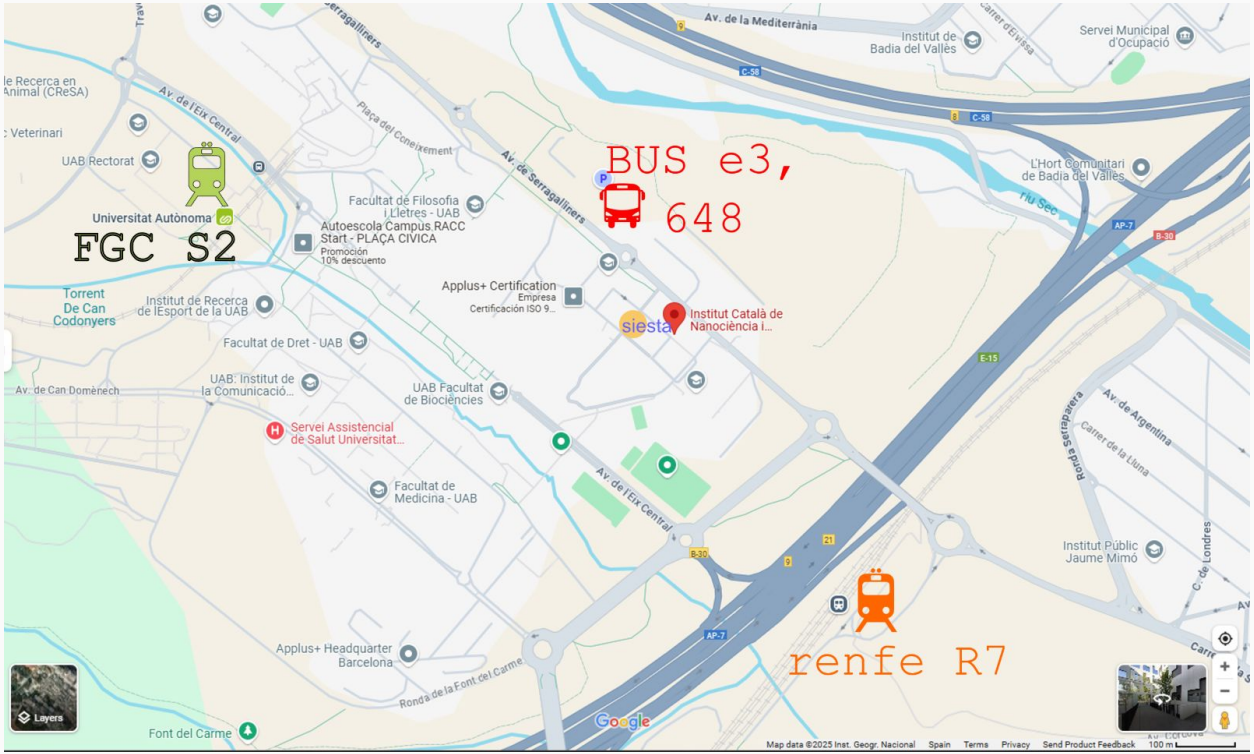
Tomorrow: Group picture!

Thursday: Poster winner announcements

Day 3: 04/06/2025	Chair: Dr. Roberta Farris	**09:00 to 10:30 - Anharmonic phonons and thermal conductivity with TDEP and SIESTA - Speakers: Prof. Matthieu Verstraete | Dr. Roberta Farris**
		10:30 to 11:00 - Coffee break
		11:00 to 13:00 - Electron-lattice interactions - Speaker: Dr. Miguel Pruneda
		13:00 to 14:00 - Lunch
		14:00 to 15:30 - Lindhard Response Function in relation to Fermi Surface Nesting - Speaker: Dr. Bogdan Guster
		15:30 to 16:30 - Roundtable on SIESTA workflows and Interoperability. Chair: Alberto García. Participants: Dr. Aldo Romero, Dr. He Xu, Dr. Roberta Farris, Dr. Yann Pouillon, Dr. Catalina Coll
		16:30 to 17:30 - Poster session & aperitif
		17:30 to 18:30 - Showcase: Using SIESTA in exascale computers: solvers for large systems, tips and tricks for GPU usage. Speaker: Alberto García
Day 4: 05/06/2025	Chair: Dr. José María Escartín	**09:00 to 09:45 - MD acceleration in SIESTA using ML - Speaker: Dr. Pol Febrer**
		09:45 to 10:30 - The role of SIESTA in future ML-based technologies. Chair: Dr. Nick Papior Participants: Dr. Alfonso Gallo, Dr. Pol Febrer, Pedro Delgado, Sara Navarro
		10:30 to 11:00 - Coffee break
		11:00 to 12:00 - Recent and future developments in SIESTA. Contributor Guidelines. Speaker: Dr. Federico Pedron
		12:00 to 13:00 - Open discussion: challenges of high throughput calculations. Unexplored areas. Chair: Dr. Federico Pedron

Practical Information

Location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Facultat de Filosofia i Lletres - UAB
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UAB Institut de la Comunicació...
UAB Facultat de Biociències
Servei Assistencial de Salut Universitat...
Facultat de Medicina - UAB
Applus+ Headquarter Barcelona
Font del Carme
Av. de la Mediterrània
Institut de Badia del Vallès
Servei Municipal d'Ocupació
L'Hort Comunitari de Badia del Vallès
Riu Sec
Av. de Serragallines
Av. de l'Eix Central
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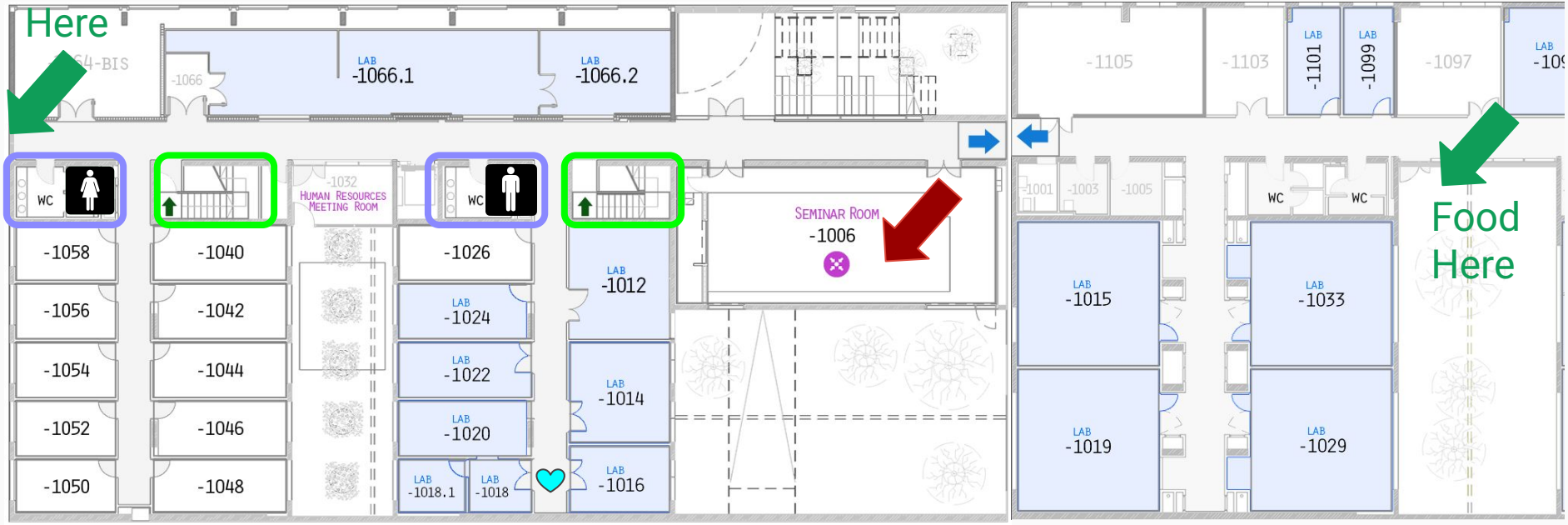
Some tips at ICN2

ICN2_Visitors, Eduroam

Some tips at ICN2

Posters Here



Social Dinner

Where:

Saona Eixample - Carrer de València 287, Barcelona

When:

Tuesday 3/June (tomorrow), *20.30*

Why?

Why siesta?™

- Really unique capabilities (for example, TS and now TS-QMMM).
- Extremely efficient in terms of computational cost (*true Green Computing*).
- Open source and in constant development
- 30 years of experience!

Can be used by a very large audience:

- It appeals to both chemists and material scientists.
- Enables quality calculations in domestic hardware.

Why this Workshop?

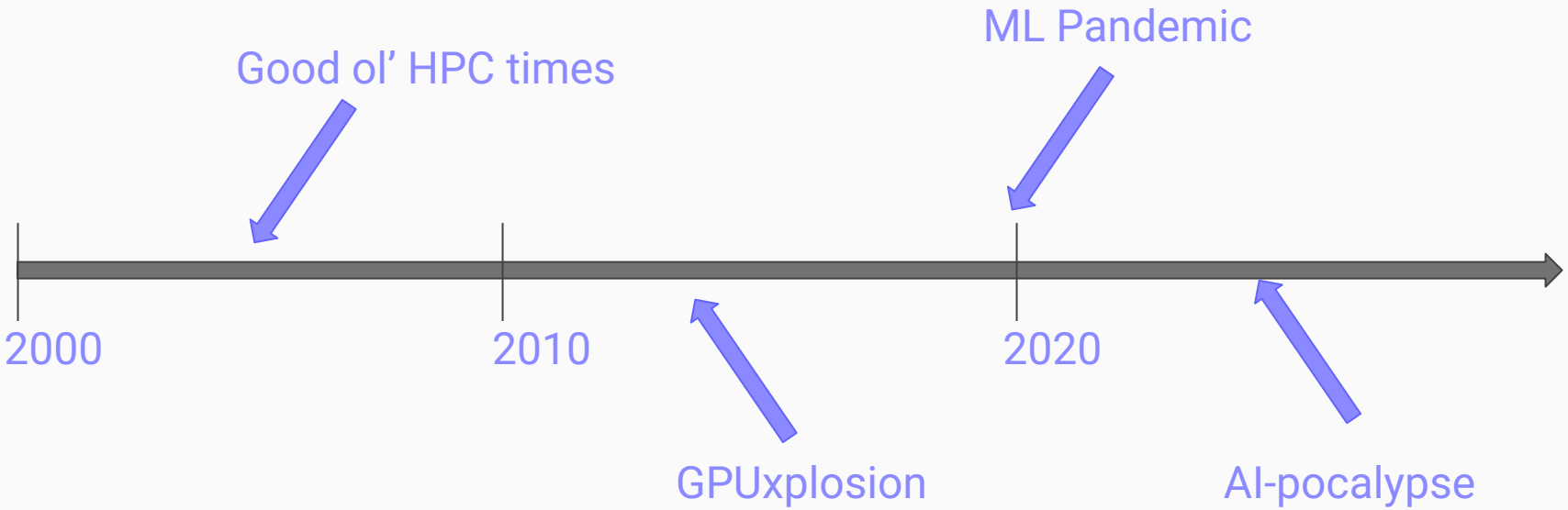
Keep these (and other) ideas in mind in the actual sessions!

siesta™ as a community

- As a user, what do you think are the main hurdles of using SIESTA?
- What could we do to engage more users and increase the reach?
- What other parts of the scientific community (outside materials science) could we interact with?

Join our Discord!

siesta™ in current research and technology



siesta™ in current research and technology

- How does SIESTA insert itself in the current environment? What about DFT in general?
- How can we best leverage the recent advances available?
- What things are now possible that previously were not?
- What else could be SIESTA doing?

Let’s get SIESTA 5.4

New release!

With conda

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

Building SIESTA 5.4 from source

Mandatory for basic MPI functionality:

- sudo apt install **gfortran cmake libopenmpi-dev liblapack-dev libscalapack-openmpi-dev**

NetCDF support, FLOOK/LUA support:

- sudo apt install **libnetcdff-dev libreadline-dev**

PEXSI support:

- sudo apt install **g++ bison flex**

Building SIESTA 5.4 from source

Get the code:

- wget https://gitlab.com/siesta-project/siesta/-/releases/5.4.0/downloads/siesta-5.4.0.tar.gz
- tar -xvf siesta-5.4.0.tar.gz
- cd siesta 5.4.0

Compile and install:

- cmake -S . -B _build -DCMAKE_INSTALL_PREFIX=/path/to/installation
  -DSCALAPACK_LIBRARY="-lscalapack-openmpi"
- cmake --build _build -j
- cmake --install _build

Learn. Discuss. Enjoy!