siesta

Advanced SIESTA Workshop 2025

CECAM Flagship and Psi-k Workshop

Barcelona, 2-5 June 2025

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Grant PCI2022-134972-2, PCI2022-134978-2 and PCI2022-135083-2 funded by

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About

The unique advantages of the SIESTA method[1][2] allow for the exploration of boundaries that are hard to be achieved by other DFT approaches. In this Workshop, we will showcase and discuss state-of-the-art research that relies on SIESTA and its interfaces with other computational tools.

Examples of these include the calculation of advanced magnetic properties (relying on TB2J[3]), thermal conductivity (via TDEP[4]), electrochemical processes (via SIESTA's own QM/MM interface[5]), potential energy surface explorations (with SIESTA/LUA) and electron-phonon coupling phenomena (with the elph interface). The usage of SIESTA in exascale and pre-exascale systems will be discussed, covering different technologies available for the calculation of electronic properties with tens of thousands of atoms. We will also include a discussion on how machine learning technologies intertwine with SIESTA, be it as a means to accelerate and improve calculations, or to use SIESTA as a provider for training data in other neural network approaches.

In this 3-day workshop, experts on the different topics will showcase current advances on their respective areas while also providing guidelines and opening the discussion for new approaches and ideas. A few selected sessions will also include short hands-on sections to further exemplify their capabilities.

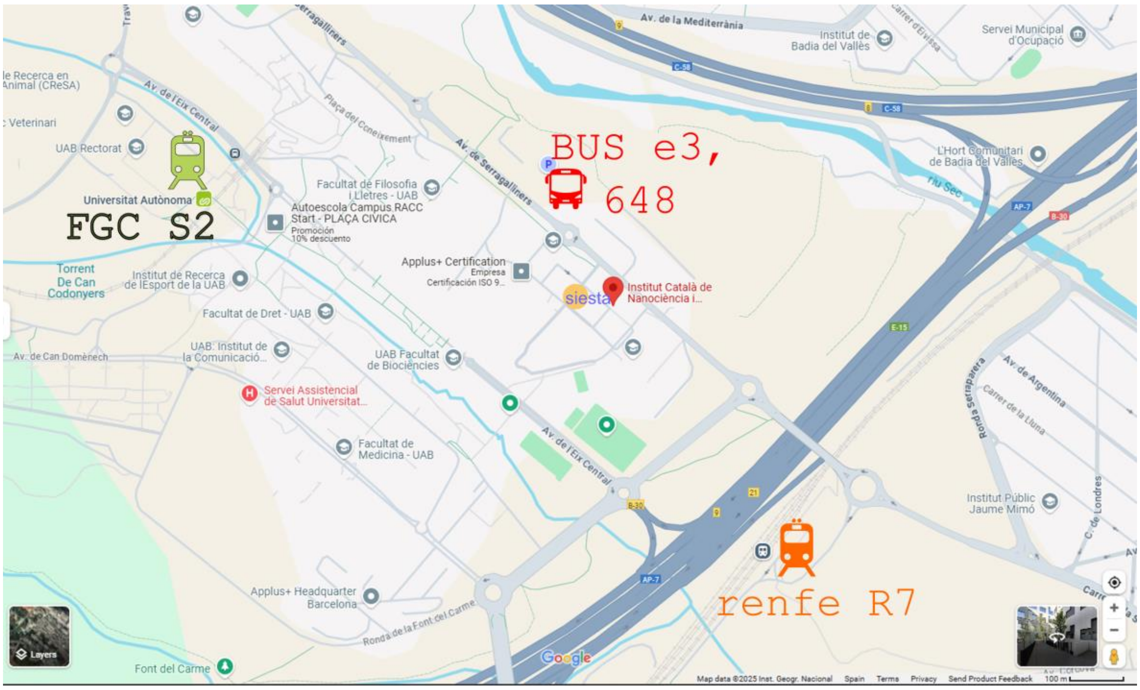
[1] J. Soler, E. Artacho, J. Gale, A. García, J. Junquera, P. Ordejón, D. Sánchez-Portal, J. Phys.: Condens. Matter, **14**, 2745-2779 (2002)
[2] A. García, N. Papior, A. Akhtar, E. Artacho, V. Blum, E. Bosoni, P. Brandimarte, M. Brandbyge, J. Cerdá, F. Corsetti, R. Cuadrado, V. Dikan, J. Ferrer, J. Gale, P. García-Fernández, V. García-Suárez, S. García, G. Huhs, S. Illera, R. Korytár, P. Koval, I. Lebedeva, L. Lin, P. López-Tarifa, S. Mayo, S. Mohr, P. Ordejón, A. Postnikov, Y. Pouillon, M. Pruneda, R. Robles, D. Sánchez-Portal, J. Soler, R. Ullah, V. Yu, J. Junquera, The Journal of Chemical Physics, **152**, (2020)
[3] X. He, N. Helbig, M. Verstraete, E. Bousquet, Computer Physics Communications, **264**, 107938 (2021)
[4] F. Knoop, N. Shulumba, A. Castellano, J. Batista, R. Farris, M. Verstraete, M. Heine, D. Broido, D. Kim, J. Klarbring, I. Abrikosov, S. Simak, O. Hellman, JOSS., **9**, 6150 (2024)
[5] C. Sanz-Navarro, R. Grima, A. García, E. Bea, A. Soba, J. Cela, P. Ordejón, Theor. Chem. Acc., **128**, 825-833 (2010)

Organisers

- Catalina Coll (Institut Català de Nanociència i Nanotecnologia (ICN2))
- José María Escartín Esteban (Institut Català de Nanociència i Nanotecnologia (ICN2))
- Roberta Farris (Institut Català de Nanociència i Nanotecnologia (ICN2))
- Federico Nicolás Pedron (Institut Català de Nanociència i Nanotecnologia (ICN2))
- Miguel Pruneda (Consejo Superior de Investigaciones Científicas (CSIC))

Practical information

- **Venue:** The workshop will take place at ICN2, in the seminar room. https://g.co/kgs/YdsTz2x . Physical registration will be open from 14.00 at ICN2 entrace.



- **Facilities:** The room will be equipped with ample sockets and tables for participants using personal laptops.

- **Poster Presentations:** There are no strict requirements regarding poster size — A0 or A1 are recommended, but you're free to choose what works best for you so long as it is in portrait orientation. We're also pleased to announce that there will be prizes for the best two posters!

- **Social Dinner:** The social dinner will be covered by the organization and will take place on Tuesday, June 3rd, at **Saona Eixample** (https://g.co/kgs/Ptr17uD)

- **Lunch:** Unfortunately, lunches will not be provided. However, there are several affordable dining options near ICN2.

- **Workshop Website:** In addition to the CECAM page, we now have a dedicated website with further details and updates throughout the event. You can access it here: https://siesta-project.org/siesta/events/Advanced_SIESTA_Workshop-2025/

- **Travel Information:** If you are arriving after the start of the workshop or leaving before it ends, please let us know your arrival and/or departure dates as this is required for funding documentation.

Program

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. Ernane 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
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

Participants (by country)

Belgium
Arsalan Akhtar (UCLouvain)
Xu He (Univeristy of Liege) - Speaker
Matthieu Verstraete (University of Liege) - Speaker
Denmark
Nick Papior (Technical University of Denmark) - Speaker
France
Perpetua Muchiri (University Paris Saclay)
Andrei Postnikov (Université de Lorraine)
Germany
Ludovica Zullo (Universität Würzburg)
Italy
Amin Alibakhshi (SISSA, Italy)
Bogdan Guster (UNINA) - Speaker
Netherlands
Arnold Kole (Utrecht University) - Speaker
Peru
Christian Solis Calero (Universidad Nacional Mayor de San Marcos)
Poland
Dorota Biernacka (Warsaw University of Technology)
Narayan Som (Warsaw University of Technology)
Spain
Anthoni Alcaraz Torres (Catalan Institute of Nanoscience and Nanotechnology)
Isaac Alcon (Universitat de Barcelona)
Emilio Artacho (Nanogune, Ikerbasque and University of Cambridge)
Aleksander Bach Lorentzen (Donostia International Physics Center)
Maria Camarasa Gomez (Centro de Física de Materiales CFM/MPC (UPV/EHU-CSIC))
Joan Cardona Olives (Universitat de Barcelona)
Catalina Coll (Institut Català de Nanociència i Nanotecnologia) - Organiser
Ernane De Freitas Martins (ICN2) - Speaker
Pedro Delgado Galindo (Universidad de Granada)
Oussama ER-RIYAHI (CIC NanoGUNE)
José María Escartín Esteban (Catalan Institute of Nanoscience and Nanotechnology (ICN2)) - Organiser
Roberta Farris (Institut Català de Nanociència i Nanotecnologia (ICN2)) - Organiser
Alfonso Gallo Bueno (University of Oviedo)
Alberto Garcia (Institut de Ciencia de Materials de Barcelona (ICMAB-CSIC)) - Speaker
Arnau Garcia Duran (Universitat de Barcelona)
Aran Garcia-Lekue (DIPC (Donostia International Physics Center)) - Speaker
Daniel García (Donostia International Physics Center)
Mónica García Mota (Simune Atomistics)
Jaime Garrido Aldea (ICN2)
Sanaz Gerivani (CIC Nanogune)

Martin Irizar (DIPC)
Javier Junquera (Universidad de Cantabria)
Álvaro López Cazalilla (Barcelona Supercomputing Center)
Karolina Milowska (CIC NanoGUNE)
Sara Navarro Rodriguez (ICN2)
Pablo Ordejon (Institut Català de Nanociéncia i Nanotecnologia - ICN2) - Speaker
Federico Nicolás Pedron (Catalan Institute of Nanoscience and Nanotechnology (ICN2)) - Organiser & speaker
Yann Pouillon (CIC NanoGUNE)
Miguel Pruneda (Consejo Superior de Investigaciones Científicas (CSIC)) - Organiser & speaker
Christian Radermacher (ICN2)
Daniel Sanchez Portal (Centro de Física de Materiales CSIC-UPV/EHU)
Jose Angel Silva Guillen (IMDEA Nanociencia)
Massimiliano Stengel (ICMAB)

Switzerland
Pol Febrer Calabozo (EPFL) - Speaker

United States
Aldo Romero (West Virginia University) - Speaker

List of posters

1. **Case-oriented machine-learning interatomic potentials using SIESTA,** *Alvaro López Cazalilla*
2. **Tuning the transition temperature of Fe(II) spin-crossover systems embedded in carbon nanohoops,** *Arnau Garcia*
3. **Development of a SIESTA Interface with atomate2 for Automated DFT Workflows,** *Arsalan Akhtar*
4. **Towards manipulation of edge states in functionalized 5-armchair graphene nanoribbons (5AGNR),** *Daniel García Pina*
5. **Robust quantum engineering of current flow in carbon nanostructures at room temperature***, Isaac Alcón*
6. **Exploring Structure-Hyperfine Coupling Relationship in Mononuclear Molecular Qubits,** *Joan Cardona*
7. **$TaTe_2$: A vast landscape of structural and electronic properties,** *Jose Angel Silva Guillen*
8. **Electronic structure of the InAs-Al interface via DFT: using ZnTe and CdSe barriers for topological Devices.** *Malcolm J.A.*
9. **Predicting accurate fundamental and excitonic properties of bulk, monolayer and surface materials from first-principles using hybrid functionals and artificial intelligence,** *María Camarasa-Gómez*
10. ***Ab initio* insights into the electronic properties of 1D and 2D porous carbon-based nanoarchitectures,** *Martin Irizar*
11. **Beyond DFT: Development of a Fe-C fusion ready potential within the NEP approach,** *Pedro Delgado,*
12. **Improved real-time propagators for a moving basis in SIESTA**, *Sanaz Gerivani,*
13. **Electrolyte Dynamics Under Electrostatically Induced Electrode Charges: Implementation and Usage as a Starting Point for TranSIESTA Calculations.** *Sara Navarro*
14. **Interfacing SIESTA with Qiskit.** *Yann Pouillon*
15. **Zandpack: A general tool for time-dependent transport simulation of nanoelectronics** *Aleksander Bach Lorentzen*

Case-oriented machine-learning interatomic potentials using SIESTA

Alvaro López Cazalilla
Barcelona Supercomputing Center (Spain)

The use of machine learning interatomic potentials (MLIP) in molecular dynamics (MD) has become a hot topic in the recent years to reproduce complex atomic scale processes. Density functional theory (DFT) codes, particularly plane-wave codes (e.g. VASP), are employed to generate a detailed dataset of atomic structures to train the interatomic potential through a machine learning algorithm. Typicially, these datasets contain a wide range of atomic configurations to cover with high-accuracy many processes, obtaining a complete reproduction of the material behaviour. However, in many cases the MLIP needed to explore a certain property of a material does not need a high accuracy in all the properties. In our work, we use open-source DFT code SIESTA (LCAO), which allows a full control of the parameters such as the accuracy in a computationally efficient way, to generate a case-oriented training dataset to create MLIPs in a relatively unsupervised manner.

In our work, we use open-source DFT code SIESTA (LCAO), which allows a full control of the parameters such as the accuracy in a computationally efficient way, to generate a case-oriented training dataset to create MLIPs in a relatively unsupervised manner.

Tuning the transition temperature of Fe(II) spin-crossover systems embedded in carbon nanohoops

Arnau Garcia, Jordi Cirera;
Universitat de Barcelona

Spin-crossover (SCO) systems are transition metal complexes in which the metal center can adopt different electronic spin states that are close in energy. This enables the molecule to switch between configurations in response to external stimuli, such as temperature or pressure. A key parameter for characterizing these systems is the transition temperature (T1/2), defined as the temperature at which both spin states coexist in equilibrium. These molecules are excellent candidates for molecular switches, making them promising for applications in molecular memory storage systems and nanoscale spintronics devices. In recent years, carbon nanostructures have attracted significant attention due to their outstanding conductive properties. In this study, we focus on a specific type of carbon nanostructure, the nanorings, whose functionalization enables them to act as ligands. The main goal of this work is to investigate SCO systems based on Fe(II) embedded in carbon nanorings, and to analyse how this affects the T1/2. Specifically, in the system [Fe(bipy[n]CPP){H2B(pz-R)2}2] (n=7-12), we have examined how variations in the nanoring size (n) and in the substituent group on the pyrazole ligand (R=H, NO2, CH3, Cl, NH2, CF3) influence the T1/2. By identifying correlations between these electronic structure modifications and the T1/2, it becomes possible to design molecules that switch at a targeted temperature. Additionally, we have explored multinuclear systems by introducing two or three metal centers into the nanorings. Dinuclear and trinuclear complexes of the types [Fe2(dibipy[n]CPP){H2B(pyz)2}4] (n=8,10,12,14) and [Fe3(tribipy[n]CPP){H2B(pyz)2}6] (n=9,12,15) were analysed to determine how the incorporation of additional metallic centers and variations in the nanoring size affect the T1/2. This study was conducted using an in-house Python code, which solves the Slichter and Drickamer model for dinuclear and trinuclear species, allowing us to predict the type of transition behaviour these systems will exhibit.

Development of a SIESTA Interface with atomate2 for Automated DFT Workflows

Arsalan Akhtar
UCLouvain

The increasing demand for accelerated materials discovery necessitates robust and automated computational workflows. Atomate2 provides a powerful, flexible framework for managing and executing complex Density Functional Theory (DFT) calculations. To broaden its applicability and leverage the unique capabilities of numerical atomic orbital basis sets, we present the development of a comprehensive interface for the SIESTA code within the atomate2 ecosystem. This work details the implementation of "builders," "flows," and "makers" tailored for SIESTA, enabling automated generation of input files, job submission, output parsing, and data management for a wide range of material property calculations. The integration of SIESTA with atomate2 facilitates high-throughput screening campaigns, systematic convergence studies, and the construction of complex multi-step workflows (e.g., relaxations followed by electronic structure or phonon calculations) using SIESTA's efficient and scalable approach. This development significantly enhances the modularity of the atomate2 platform and opens new avenues for computational materials science by combining SIESTA's strengths with established workflow automation tools, thereby contributing to the synergistic advancement of materials informatics and simulation.

Towards manipulation of edge states in functionalized 5-armchair graphene nanoribbons (5AGNR)

Daniel García Pina
Donostia International Physics Center (DIPC)

In the last years, on-surface synthesis techniques have granted access to unprecedented atomistic control over the of bottom-up fabrication graphene nanoribbons (GNRs). This highly precise experimental platform has given rise to multiple studies in these systems regarding topological properties [1], chemical substitution [2,3], novel morphological structures [4] , etc. In this work, we use Density Functional Theory calculations to gain insights into the electronic structure and topological properties of several functionalized GNRs. The systems considered consist of 5 carbon atoms wide armchair GNRs (5AGNRs) with OH and F groups attached to their edges. We study the effect of these radicals in the physical structure, the wavefunctions and the topology of the system. We find that, while retaining their overall structure, functionalization with chemical groups of different electron affinities, different orientations and at different concentrations can change the topology of the system. Our results might be of interest for the engineering and development of new experiments regarding the topological and magnetic properties of these materials.

References

[1] J. Li, S. Sanz, N. Merino-Díez et al., Nat Commun 12 (2021) 5538

[2] N. Friedrich et al., ACS Nano 16, 9, (2022) 14819-14826

[3] N. Friedrich et al., Phys. Rev. Letters 125 (2020) 146801

[4] S. Sanz, N. Papior, G. Giedke, D. Sanchez-Portal, M. Brandbyge, T. Frederiksen, Phys. Rev. Letters 129 (2022) 037701

"Robust quantum engineering of current flow in carbon nanostructures at room temperature".

Gaetano Calogero, Isaac Alcón, Onurcan Kaya, Nick Papior, Aron W. Cummings, Mads Brandbyge, Stephan Roche.
Universitat de Barcelona

Bottom-up on-surface synthesis enables the fabrication of carbon nanostructures with atomic precision. Good examples are graphene nanoribbons (GNRs), 1D conjugated polymers, and nanoporous graphenes (NPGs), which are gathering increasing attention for future carbon nanoelectronics. A key step is the ability to manipulate current flow within these nanomaterials. Destructive quantum interference (QI), long studied in the field of single-molecule electronics, has been proposed as the most effective way to achieve such control with molecular-scale precision. However, for practical applications, it is essential that such QI-engineering remains effective near or above room temperature. To assess this important point, here we combine large-scale molecular dynamics simulations and quantum transport calculations and focus our study on NPGs formed as arrays of laterally bonded GNRs. By considering various NPGs with different inter-GNR chemical connections we disentangle the different factors determining electronic transport in these carbon nanomaterials at 300 K. Our findings unequivocally demonstrate that QI survives at room temperature, with thermal vibrations weakly restricting current flow along GNRs while completely blocking transport across GNRs. Our results thus pave the way towards the future realization of QI-engineered carbon nanocircuitry operating at room temperature, which is a fundamental step towards carbon-based nanoelectronics and quantum technologies.

Exploring Structure-Hyperfine Coupling Relationship in Mononuclear Molecular Qubits

Joan Cardona, Silvia Gómez-Coca, Eliseo Ruiz;
Universitat de Barcelona

A key challenge for spin qubit technologies is achieving long coherence times at room temperature. Molecular qubits lose their information-storing ability (orientation) due to interactions with the environment (known as T1 or spin-lattice relaxation) and amongst other spins (T2 or spin-spin relaxation). Thus, T2 time is a fundamental parameter for spin coherence, since in most systems is much shorter than T1 in a low temperature regime. In the field of spin qubits, achieving coherence times in the range of 0.1 to 1 millisecond, as demonstrated by Freedman et al. , is considered a desirable outcome. High T2 values are attributed to the influence of hyperfine coupling, the interaction between the electronic and nuclear spins of the same atom. Given the pivotal role of hyperfine coupling, it is of peak interest in our research to further study and unravel thoroughly its underlying mechanisms. Similar to how molecular structural design dictates the function of a molecule, hyperfine coupling profoundly influences qubit coherence. Our focus is to investigate the structure - hyperfine coupling relationship as it is crucial for optimizing qubit design and enhancing coherence. Furthermore, recent research suggests a deeper significance of hyperfine coupling as a fine-tuning parameter for achieving magnetic noise immunity to a certain degree in qubit clock transitions, leading to significant coherence improvements.

$TaTe_2$: A vast landscape of structural and electronic properties.

Jose Angel Silva Guillen
IMDEA Nanociencia

Transition metal dichalcogenides feature a wide range of physical and electronic properties that range from semiconducting to metallic. Moreover, they can host many-body correlated states such as superconducting phases, Mott insulator phases and charge density waves (CDW) which have brought a lot of excitement to the scientific community. The most common polymorph of group VI TMDC is the 2H since it is the most stable one. Despite that, other structures can be found in nature, and thanks to the development of new growing techniques, experimentalists can grow large samples of these structures. Although sulphur and selenium compounds have been thoroughly studied in the past years, tellurium based have been less studied. Interestingly, group V Te-based single-layers are catching attention lately since the absence of Te-Te interlayer interactions changes the electron transfer compared to the bulk or multi-layer cases and new structures and electronic properties can be found [1,2]. In this work [3], we study the structural and electronic properties of single-layer TaTe2 using first-principles calculations [4]. We find that it presents a large number of possible structures which are very close in energy. We study in detail the formation of these structures and give a possible mechanism for their formation. Moreover, we study their electronic properties in a comprehensive way. References

[1] I. Di Bernardo, et. al., Small 202300262 (2023).
[2] J. Hwang, et al., Advanced Materials 202204579 (2022).
[3] J.A. Silva-Guillen, E. Canadell. Submitted (2024).
[4] A. García., J. Chem. Phys. 152, 204108 (2020).

Electronic structure of the InAs-Al interface via DFT: using ZnTe and CdSe barriers for topological Devices.

Malcolm J.A. Jardine, Derek Dardzinski, Chris J. Palmstrom, Moira Hocevar, Vladimir N. Strocov, Sergey M. Frolov, Noa Marom.
Carnegie Mellon University

Understanding the effects of interfacing materials is pivotal to the design of semiconductor, spintronic, and quantum devices. We study the InAs/ZnTe,CdSe/Al interface via density functional theory (DFT). InAs based systems are popular for Majorana setups for topological quantum computing. To supply the necessary superconducting affect this is interfaced with Al. However, this interfacing can lead to detrimental effects in the InAs, so the favorably lattice matched materials of ZnTe and CdSe are explored as a tunnel barrier between the InAs/Al interface. The PBE+U method is used, with the Hubbard U parameters found via a machine-learned Bayesian optimization algorithm, allowing the simulation of large interfaces. We discuss effects such as band offsets at the interfaces, metal induced gap states (MIGS) and the effects of varying the barrier thickness. We also study the comparison of our CdTe and αSn DFT data with experimental ARPES data, utilizing the tools of bulk and z-unfolding to visualize our data.

Predicting accurate fundamental and excitonic properties of bulk, monolayer and surface materials from first-principles using hybrid functionals and artificial intelligence

María Camarasa-Gómez
Centro de Física de Materiales (CFM-MPC) CSIC-UPV/EHU

GW and the Bethe-Salpeter equation are considered to be the state-of-the-art techniques to determine the electronic structure and the optical absorption spectra of low-dimensional systems and bulk materials. Nevertheless, they are very computational demanding, being almost prohibitive for large supercells and systems with broken spatial symmetry, as the ones commonly employed for simulating reconstructed surfaces and van der Waals (vdW) monolayers. Therefore, it is of wide interest to develop alternative methods which allow for the accurate calculation of electronic and optical properties for these systems. This challenge can be overcome using density functional theory with a new generation of optimally-tuned screened range-separate hybrid functionals, yielding a level of accuracy comparable to that of ab initio many-body perturbation theory with a significant reduction of the computational cost. In this contribution, we demonstrate that, by integrating ground-state and time-dependent density functional theory, specific hybrid functionals can accurately predict, fundamental and optical gaps of monolayer and bulk systems [1], surface-states [2], as well as the band structures and optical absorption spectra of vdW materials [1], and projected band structures of surfaces [2].

[1] M. Camarasa-Gómez, S. E. Gant, G. Ohad, J. B. Neaton, and L. Kronik, npj Comp. Mat. 10, 288 (2024)

[2] F. Sagredo, M. Camarasa-Gómez, F. Ricci, A. Champagne, L. Kronik, and J. B. Neaton (submitted, 2025)

Ab initio insights into the electronic properties of 1D and 2D porous carbon-based nanoarchitectures

Martin Irizar
DIPC, EHU-UPV

In recent years, a wide selection of atomically-precise carbon-based nanoarchitectures has been created using on-surface synthesis (OSS) techniques. [1,2] Remarkably, it is now possible to obtain carbon-based materials using allotropes other than graphene, such as biphenylene. [3] This emerges as a new degree of freedom to tune the electronic properties of such 1D and 2D materials. In this work, we employ Density Functional Theory (DFT) to explore how the electronic properties of 1D and 2D carbon- based nanoarchitectures are modified by the inclusion of graphene-like and biphenylene- like units. In particular, we focus on porous 12-atoms-wide armchair graphene nanorribons (12-PGNR), and on the 2D nanoporous networks that would emerge from their lateral fusion. The nature of this lateral fusion, either graphene-like or biphenylene- like, greatly affects the electronic properties of the resulting 2D system. Our results will be useful to interpret Scanning Tunneling Microscope (STM) and Atomic Force Microscope (AFM) experiments performed by our collaborators.

Beyond DFT: Development of a Fe-C fusion ready potential within the NEP approach,

Pedro Delgado, Pablo Canca, María José Caturla, Blanca Biel.
Consorcio IFMIF-DONES España

In recent years, there has been a flourishing in the development of new techniques to study materials. One of these techniques is the use of machine learning interatomic potentials (MLIAPs), instead of traditional interatomic potentials, to perform molecular dynamics simulations (MD). The current classical potentials lack the accuracy of quantum approaches such as Density Functional Theory (DFT) but MLIAPs combines the precision of the quantum approaches with the speed and efficiency of classical potentials. In the field of fusion, MD is useful to obtain key parameters for other methods such as Montecarlo simulations, as well as characterizing relative low energy neutron induced defect cascades with the primary knock-on atom approach. The use of accurate potentials is thus key to correctly describe the multiscale simulations needed in the characterization of irradiated materials. These MLIAPs will be useful to compare with experimental data obtained in facilities such as IFMIF-DONES In this work we developed and tested a potential for Fe-C systems based on the Neuroevolutional Potential (NEP) [1] method due to its high accuracy and efficiency. We employed a database of 30000 Fe-C structures for the fitting of the potential and added a ZBL potential [3] region to correctly characterize the short interaction in cascades. With this MLIAP we study common defective structures found on irradiated steels and compare the results with already existing classical potentials. [1] Z. Fan, et al, Phys. Rev. B. 104, 2021 104309. [2] J.F. Ziegler et al., Pergamon, Volume 1, 1985.

Improved real-time propagators for a moving basis in SIESTA,

Sanaz Gerivani, Emilio Artacho.
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When dealing with the time-dependent Schrödinger equations for a non-orthogonal basis set in systems with the basis set that evolve over time, it is essential to account for the time-dependent basis set evolution. In SIESTA code the Crank-Nicholson algorithm has been used quite successfully to solve these equations, and it includes two different approaches for dealing with the systems with moving basis set, Löwdin orthonormalization and affine connection method [4]. Lowdin orthonormalization is based on Sankey and collaborators work which has shown good performance for low-velocity dynamics. The affine connection method extends the time-dependent Schrödinger equation to include the evolving basis effects through the D-matrix. This modifies the Hamiltonian as H-iD, where D represents the time evolution of basis and introduces a gauge-like potential that modifies the dynamics. While the affine connection method offers superior accuracy for high-velocity dynamics and electronic stopping power, it does not strictly conserve unitarity for arbitrary time steps. To address these challenges our goal is to develop advanced multiscale methodologies for the quantum evolution of electrons and nuclei within the SIESTA framework. These methods aim to extend the capabilities of existing techniques, such as those we already have for Löwdin orthonormalization, extrapolation and two step schemes, enabling the use of larger time steps, to achieve high computational efficiency and optimize simulation times. Larger time steps would allow for the exploration of longer time-scale phenomena, such as the thermalization processes and quantum nuclear dynamics that are central to the study of irradiated systems.

Electrolyte Dynamics Under Electrostatically Induced Electrode Charges: Implementation and Usage as a Starting Point for TranSIESTA Calculations

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Understanding the electrode/electrolyte interface at the atomistic level is essential for electrochemical processes like corrosion and energy storage, but simulations are often limited by system size, time scales, and the out-of-equilibrium nature imposed by external potentials. Within the SIESTA DFT framework, some of these challenges are addressed using non-equilibrium Green's functions (NEGF) to include external bias and a hybrid QM/MM scheme to model large systems. However, NEGF-QM/MM simulations remain limited to short time scales (~0.1 ns), which are insufficient to equilibrate the electrolyte response. To overcome this, we implement the Siepmann–Sprik method, which models induced electrode charges classically, allowing the electrolyte to equilibrate under potential and generate realistic initial configurations for DFT. Our results show strong agreement with NEGF-QM/MM benchmarks while reducing simulation times by over a factor of 10, providing an efficient and accurate approach for simulating electrochemical interfaces.

Interfacing SIESTA with Qiskit

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We are exploring the solution of electronic structure problems with highly-correlated electrons in an embedding setting, for possibly-large condensed matter systems with many weakly correlated electrons containing an embedded set of highly-correlated electronic states. The latter defines an active space to be addressed by a full many-body solution on quantum computers, while the former is addressed with SIESTA at the density-functional theory level on a classical high-performance computer. The highly-correlated problem represents one of the most natural applications of quantum computing with a clear long-term advantage over classical computing, and the hybrid combination offers wide applicability in contexts from molecular biology to materials. We are currently integrating both programs and approaches within the SIESTA-QCOMP software suite, using the Variational Quantum Eigensolver (VQE) algroithm, which allowed proof-of-concept and early demonstrative calculations. A large-scale calculation is underway involving over 20 qubits, as affordable with VQE. We now want to extend and generalise the power of the hybrid setup by incorporating the Sample-based Quantum Diagonalisation (SQD) solver, which will scale up to more than 60 qubits, already in the quantum utility remit. In addition to coding, testing and preparing a release, the project aims at demonstrating the power of this approach for an envisaged iron porphyrin molecule in a haemoglobin environment with an active space of the 3d orbitals of Fe, the valence ones of O2 and of neighbouring N anchors. The combined software will be integrated into SIESTA and will be applicable to many contexts addressable with embedding. It will also set the basis for a long-term initiative ensuring the interoperability of different DFT codes with quantum computing environments, codename QCOMP4DFT.

Zandpack: A general tool for time-dependent transport simulation of nanoelectronics

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A python package to simulate time-dependent electron transport in open systems using nonequilibrium Greens functions[1] has been developed. It employs the auxiliary mode method together with an eigen-decomposition[2] of the electrode level-width functions to allow one to simulate large device regions in real time. Using this method, the device region can be described up to the TD-DFT level or below, allowing one to simulate excitation phenomenon, transient states as the open system is driven by strong, transient fields. Three examples are modeled; a simple tight-binding model with a one-site mean-field Hubbard term, a three-electrode STM-like measurement on an AGNR nanoribbon and a gold break junction. In all examples a transient THz electric field, which is based on experimental data, is used.