

BOOK OF ABSTRACTS

Materials Science from First Principles

Organizers:

Michele Casula, CNRS and Sorbonne Université, Paris, France

Daniele Varsano, CNR Institute of Nanoscience, Modena, Italy

Edoardo Di Napoli, Forschungszentrum Jülich, Germany

Giacomo Giorgi, University of Perugia, Italy

Pablo Ordejón, Catalan Institute of Nanoscience and Nanotechnology - ICN2

France Boillod-Cerneau, CEA Fundamental Research Department, Saclay, France

November 3–7

Sorbonne University, Paris, France

Supported by:



Contents

1 HANAMI-CECAM Materials Science Event Program	2
2 Poster Session Abstracts	9
3 Workshop Presentation Abstracts	28
4 Practical information	52
Acknowledgements	56

HANAMI-CECAM Materials Science Event Program

Skill-building

Day 1: November 3 (Monday)

08:30 – 08:45 General Registration (Amphi Durand)

08:45 – 09:00 Opening Remarks (Amphi Durand)

Density Functional Theory for Materials Modeling

09:00 – 10:40 P. Ordejón: *Density Functional Theory and the SIESTA code* (Amphi Durand)

10:40 – 11:00 ☕ Coffee Break (SCAI)

11:00 – 11:45 P. Ordejón: *Density Functional Theory and the SIESTA code (cont'd.)* (Amphi Durand)

11:45 – 12:30 E. di Napoli: *Linear Algebra Use in DFT Codes* (Amphi Durand)

12:30 – 14:00 🍴 Lunch Break (SCAI)

14:00 – 15:30 A. Alcaraz and P. Ordejón: *Practical Sessions with SIESTA* (UFR Physique: Corridor 22-23, 1st floor, computer rooms 109-111)

15:30 – 16:00 ☕ Coffee Break (UFR Physique: Corridor 22-23, 1st floor, room 103)

16:00 – 17:40 A. Alcaraz and P. Ordejón: *Practical Sessions with SIESTA* (UFR Physique: Corridor 22-23, 1st floor, computer rooms 109-111)

17:40 – 📄🍷 **Poster Session and Cocktails** (IMPMC institute: Corridor 23-24, 4th floor, conference room 402)

Day 2: November 4 (Tuesday)

Quantum Monte Carlo Methods for Accurate Materials Simulations

08:30 – 09:00	K. Nakano: <i>Overview of the TURBORVB code</i> (<i>Amphi Durand</i>)
09:00 – 10:40	M. Casula: <i>Introduction to Quantum Monte Carlo: stochastic integration and the correlated wave function</i> (<i>Amphi Durand</i>)
10:40 – 11:00	☕ Coffee Break (<i>SCAI</i>)
11:00 – 12:00	M. Casula: <i>Variational Monte Carlo and wave function optimization</i> (<i>Amphi Durand</i>)
12:00 – 12:30	Edoardo Di Napoli and Clément Richefort: <i>Linear Algebra Use in QMC Codes: the conjugate gradient method</i> (<i>Amphi Durand</i>)
12:30 – 14:00	🍴 Lunch Break (<i>SCAI</i>)
14:00 – 15:30	K. Nakano and M. Casula: <i>Practical Sessions with TurboRVB: First steps: the hydrogen molecule and the resonating valence bond (RVB) wave function</i> (<i>UFR Physique: Corridor 22-23, 1st floor, computer rooms 109-111</i>)
15:30 – 16:00	☕ Coffee Break (<i>UFR Physique: Corridor 22-23, 1st floor, room 103</i>)
16:00 – 17:40	K. Nakano and M. Casula: <i>Practical Sessions with TurboRVB: The benzene molecule as RVB ring and the diffusion Monte Carlo method</i> (<i>UFR Physique: Corridor 22-23, 1st floor, computer rooms 109-111</i>)

Day 3: November 5 (Wednesday)

Many-Body Perturbation Theory and the GW Approximation

- 08:30 – 08:50** D. Varsano: *Overview of the Yambo code* (Amphi Durand)
- 08:50 – 09:50** A. Ferretti: *Many Body Perturbation Theory and the GW approximation.* (Amphi Durand)
- 09:50 – 10:30** C. Attaccalite: *Optical properties & the Bethe Salpeter equation* (Amphi Durand)
- 10:30 – 10:50** ☕ Coffee Break (SCAI)
- 10:50 – 11:30** D. Varsano: *GW in practice* (Amphi Durand)
- 11:30 – 12:00** C. Richefort: *Linear Algebra Use in MBPT Codes* (Amphi Durand)
- 12:00 – 14:00** 🍴 Lunch Break (SCAI)
- 14:00 – 15:30** Practical Sessions with Yambo: *First steps: a walk through from DFT to optical properties* (UFR Physique: Corridor 22-23, 1st floor, computer rooms 109-111)
- 15:30 – 16:00** ☕ Coffee Break (UFR Physique: Corridor 22-23, 1st floor, room 103)
- 16:00 – 17:40** Practical Sessions with Yambo: *A tour into the GW approximation* (UFR Physique: Corridor 22-23, 1st floor, computer rooms 109-111)
- 20:45 –** 🍷 🚤 **Conference Dinner on the Boat** for all registered participants: [Diner croisière Eiffel, boarding at the Alexandre III bridge](#)

Workshop

Workshop Day 1: November 6 (Thursday) (Amphi Charpak)

08:30 – 08:45 Workshop Registration

08:45 – 09:00 Workshop opening remarks

Pushing the Boundaries of Large-Scale Simulations

Chair: Luigi Genovese

09:00 – 09:45 **Ayako Nakata** (NIMS, Tsukuba, Japan)

Large-scale DFT calculations on nano-scale metallic materials

09:45 – 10:10 **Laura Ratcliff** (School of Chemistry, University of Bristol, UK)

Excitations in Large Systems using Transition-Based Constrained DFT

10:15 – 10:40 **Miguel Pruneda** (CINN-CSIC, Oviedo, Spain)

Electron-phonon coupling at interfaces and grain boundaries from first principles calculations

10:40 – 11:00 ☕ **Coffee Break**

Recent Advances in Linear Algebra Libraries for Materials Science

Chair: Edoardo Di Napoli

11:00 – 11:45 **Toshiyuki Imamura** (RIKEN-CCS, Kobe, Japan)

Impact of MxP on Dense Eigenvalue Computation

11:45 – 12:10 **Clément Richefort** (Jülich Supercomputing Centre, Germany)

Expanding ChASE functionalities to solve for the Bether-Salpeter equation for pseudo-Hermitian Hamiltonians

12:10 – 12:35 **Laura Grigori** (EPFL, Lausanne, Switzerland)

TBA

12:35 – 14:00 🍴 **Lunch Break** (For speakers and HANAMI members lunch at the campus restaurant L'Ardoise)

Electronic Structure and Total Energy with Many-Body Methods

Chair: Daniele Varsano

- 14:00 – 14:45 Takao Kotani** (Tottori University, Japan)
High-throughput Quasiparticle self-consistent GW
- 14:45 – 15:10 Maria Hellgren** (IMPMC, Sorbonne Université, Paris, France)
Self-consistent RPA and optimized hybrid functionals for solids
- 15:10 – 15:35 Vitaly Gorelov** (LSI, École Polytechnique, Palaiseau, France)
Computing Observables with Quantum Monte Carlo from Excitations to One-Body Reduced Density Matrices
- 15:35 – 16:00 ☕ Coffee Break**

Electronic and Optical Properties of Innovative Materials

Chair: Giacomo Giorgi

- 16:00 – 16:45 Maurizia Palumbo** (University of Rome Tor Vergata, Italy)
First-Principles Insights into the Opto-Electronic Properties of Novel 2D and Layered Materials
- 16:45 – 17:10 Claudio Attaccalite** (CINaM Marseille, France)
Non-linear Response Functions from Real-Time Simulations
- 17:10 – 17:35 Michele Amato** (LPS, Université Paris-Saclay, France)
Optical Absorption in Hexagonal-Diamond Si and Ge Nanowires: Insights from STEM-EELS and ab initio Theory
- 17:35 – 18:00 Claudio Quarti** (University of Mons, Belgium)
Simulating the Optical Properties of Solids Using ab initio BSE: There Is More than Meets the Eye
- 19:30 – 🍷 Conference Dinner** at [La Coupole \(102 Bd du Montparnasse, 75014 Paris\)](#) for speakers and HANAMI members

Workshop Day 2: November 7 (Friday) (Amphi Charpak)

Modelling and Simulation of Energy Materials

Chair: Alessandro Pecchia

- 08:30 – 09:15** **Azusa Muraoka** (Japan Women's University, Japan)
Vibronic Pathway Engineering for Efficient Exciton Separation in High-Efficiency Nonfullerene OSCs
- 09:15 – 09:40** **George Volonakis** (Université de Rennes, France)
Next-Generation Perovskites and Inspired Energy Materials from First Principles
- 09:40 – 10:05** **Aran García Lekue** (DIPC, San Sebastián, Basque Country, Spain)
1D and 2D Molecular Nanoarchitectures: Electronic Insights from DFT-Based Simulations
- 10:05 – 10:30** ☕ **Coffee Break**

Machine Learning for Materials Research

Chair: Pablo Ordejón

- 10:30 – 11:15** **Terumasa Tadano** (NIMS, Tsukuba, Spain)
First-Principles and Data-Driven Approaches for the Computational Design of Functional Heusler Alloys
- 11:15 – 11:40** **Markus Holzmann** (LPMMC, Université Grenoble-Alpes, France)
Exploring Zero-Temperature Phase Diagrams with Neural-Network Quantum States
- 11:40 – 12:05** **Alessandra Serva** (PHENIX, Sorbonne University, France)
Modelling Electrolytes for Energy Storage Applications via Machine-Learning-Based Simulations
- 12:05 – 12:50** **Tomomi Shimazaki** (Yokohama City University, Japan)
Simulation, theory, and machine learning approaches for investigating materials and molecular systems.
- 12:50 – 14:00** 🍴 **Lunch Break** (For speakers and HANAMI members lunch at the campus restaurant L'Ardoise)

Green's Function Methods for Spectroscopy

Chair: Michele Casula

14:00 – 14:45 **Lucia Reining** (LSI, École Polytechnique, Palaiseau, France)

Effective Interactions in Many-Body Perturbation Theory

14:45 – 15:10 **Andrea Ferretti** (CNR Nano, Modena, Italy)

Efficient Many-Body Perturbation Theory Calculations of (Doped) 2D Materials: Applications to ARPES and EELS Spectroscopies

15:10 – 15:35 **Valerio Olevano** (Institut Néel, Grenoble, France)

Green's Function Approaches to Spectroscopy in Photovoltaic Organic Molecules and Photosynthesis (Chlorophyll A and B in LHC II)

15:35 – 16:00 **Fabien Bruneval** (CEA Saclay, France)

Green's Functions beyond the GW Approximation: Still an Open Challenge

Poster Session Abstracts

Poster #1: Non-Centrosymmetric Hexagonal Buckled Monolayers: A Platform for Strain-Tunable Valleytronics

Authors: Fathima Is and Abir De Sarkar*

Affiliation: Institute of Nano Science and Technology, Knowledge City, Sector 81, Mohali, Punjab-140306

Abstract: In the era of information explosion and artificial intelligence, energy-efficient and high-speed computational resources have become prerequisites. Nanomaterials, especially atomically thin 2D materials, introduce new paradigms to overcome the miniaturization challenges. Valleytronics is an emerging field; an additional quantum degree of freedom called valley can be manipulated in certain materials to store and process information. Berry curvature is a geometric property of the electronic band structure that acts as a magnetic field in momentum space, determining the Valley Hall effect. In non-magnetic materials, valley polarization can be induced externally through optical pumping. The present study highlights the potential by exploring valleytronic properties in various buckled hexagonal monolayers. The spin splitting obtained for the valence band is 58 meV and 72 meV for SnSi and SnGe, respectively, and is comparable to the well-studied transition-metal dichalcogenides (TMDCs). On the other hand, the orbital-projected band structures reveal that p-orbitals contribute to the band edges. We further demonstrate that applying strain can enhance Berry curvature in SnS monolayer, paving the way for groundbreaking advancements in emerging electronic applications.

References:

1. Fathima I. S., R. Ahammed, P. Nandi, A. Rawat, and A. De Sarkar, "Compressive strain-induced enhancement in valley polarization in β -phosphorene-like SnS monolayers," *Applied Surface Science* 611, 155675 (2023).
2. M.K. Mohanta, Fathima I. S., and A. De Sarkar, "Valley Hall effect in graphene-like SnX (X= Si, Ge) buckled monolayers with high charge carrier mobility and low lattice thermal conductivity," *Phys. Rev. B* 107(3), 035429 (2023)

Poster #2: Multichannel Dyson equation: 3-body Green's functions for the investigation of molecular spectra

Authors: Stefano Paggi

Affiliation: Université de Toulouse

Abstract: We present the multichannel Dyson equation (MCDE)[1], which couples two or more independent-particle n -body Green's functions through a multichannel self-energy. In particular, the method couples a one-body Green's function with a three-body Green's function to simulate photoelectron spectroscopy. Conventional Dyson equation approaches typically start from the one-body Green's function and include satellite excitations through a complicated dynamical one-body self-energy. In contrast, the MCDE incorporates correlation effects already at the independent-particle level, allowing for a static multichannel self-energy. The MCDE is exact up to second order in the interaction and includes many higher-order diagrams to describe screening and other correlation effects. This formalism overcomes key shortcomings of standard approaches such as GW, which suffers from self-screening and fails to reproduce the satellites in the spectral function of the Hubbard dimer. The MCDE is exact for the standard Hubbard dimer[2] and yields very accurate results for hydrogen-molecule-like models[3]. Here, we present results for a H₂-like molecule and Neon.

References:

[1] Riva, Romaniello, Berger, Phys. Rev. B 110, 115140

[2] Riva, Romaniello, Berger, Phys. Rev. Lett. 131, 216401

[3] Paggi, Berger, Romaniello, J. Chem. Phys. 163, 154109 (2025)

Poster #3: Excitonic Landscape in MoS₂ and MoSe₂ Homobilayers: A First-Principles Study Using GW-BSE

Authors: Purushothaman Mannivannan

Affiliation: University of Antwerp

Abstract: This work presents a first-principles investigation of the excitonic properties in MoS₂–MoS₂ and MoSe₂–MoSe₂ bilayer systems. Using GW-corrected band structures and Bethe–Salpeter Equation (BSE) calculations performed with the YAMBO code. We analyze the low-energy excitations and classify them as direct/indirect, and intralayer/interlayer/hybrid types of excitons. Additionally, we explore the impact of biaxial strain on the excitonic landscape, aiming to understand the tunability of exciton types and binding energies in these homobilayers. Our results provide insight into excitonic transitions in 2D TMD bilayers, highlighting their relevance for tunable optoelectronic and valleytronic devices.

Poster #4: Localized Spin-State Transitions in the Optical Absorption Spectrum of Cr-doped GaN.

Authors: Masoud Mansouri

Affiliation: Universidad Autónoma de Madrid

Abstract: Using a hybrid density functional, we study the electronic, magnetic, and neutral excitations of the paradigmatic Cr-doped GaN solid. Our results indicate that the $\sim 1\%$ doped wurtzite GaN crystal retains the semiconducting nature of the host, associated with a magnetic moment of $3 \mu_B$. As a consequence of Cr doping, additional hybridized bands are formed within the intrinsic bandgap of GaN, leading to a considerable bandgap narrowing by 1.4 eV and new low-energy optical transitions. Our results indicate dark Cr d-d transitions at very low energy (0.5-0.7 eV), followed by bright transitions in the visible energy range (1.8-2.2 eV). Characterization of the electron-hole pairs suggests that the latter originates from the internal transitions among hybridized $\text{Cr}_d\text{-N}_p$ states. With the existence of these new optical features within the visible energy window, one can expect an enhancement to the photoelectric conversion efficiency of GaN upon Cr-doping, in addition to applications in spintronic devices.

Poster #5: Exploring the Impact of Electron-Phonon and Impurity-Phonon Interactions on Heat Transport in Heavily Doped Silicon: A First-Principles Study

Authors: Raja Sen (1), Nathalie Vast (3), Jelena Sjakste (3), and Lorenzo Paulatto (2)

Affiliations: (1) SATIE, ENS Paris-Saclay et Université Paris-Saclay, UMR 8029, 4 avenue des Sciences, 91190 Gif-sur-Yvette, France, (2) Sorbonne Université, Museum National d'Histoire Naturelle, UMR CNRS 7590, Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie, 4 place Jussieu, F-75005 Paris, France, (3) Laboratoire des Solides Irradiés, CEA-DRF-IRAMIS, École Polytechnique, CNRS UMR 7642, Institut Polytechnique de Paris, 91120 Palaiseau, France

Abstract: A detailed understanding of heat transport mechanisms in doped semiconductors is essential for optimizing their thermoelectric performance and improving heat management in micro- and nanoscale devices. While electron-phonon (el-ph) and electron-impurity interactions are well-studied in the context of electron transport in semiconductors [1,2], research on the impact of el-ph and phonon-impurity (ph-imp) interactions on phonon lifetimes and, consequently, on lattice thermal conductivity, remain rare. In this presentation, I will show our recent work, which explores the influence of el-ph and ph-imp scattering on the lattice thermal conductivity of heavily doped silicon [3], using density functional theory-based first-principles methods. Our findings show that at moderate carrier concentrations (10^{17} cm^{-3}) and room temperature, phonon scattering by electrons is the main mechanism behind the reduction of thermal conductivity in doped silicon. However, at lower temperatures or higher doping levels (10^{21} cm^{-3}), both el-ph and ph-imp scattering significantly contribute to reducing the lifetimes of low-frequency phonons, which leads to further decreases in the thermal conductivity of doped silicon. Our results show good agreement with experimental thermal conductivity data for silicon across the full range of doping levels and temperatures.

References:

1. R. Sen, N. Vast, and J. Sjakste, "Role of Dimensionality and Size in Governing the Drag Seebeck Coefficient of Doped Silicon Nanostructures: A Fundamental Understanding" *Phys. Rev. B* 108, L060301, (2023). (Highlighted as Editors' Suggestion)
2. R. Sen, N. Vast, and J. Sjakste, "Hot Electron Relaxation and Energy Loss Rate in Silicon: Temperature Dependence and Main Scattering Channels" *Appl. Phys. Lett.* 120, 082101, (2022).
3. J. Sjakste, M. Markov, R. Sen, G. Fugallo, L. Paulatto, and N. Vast, "Occurrence of the Collective Ziman Limit of Heat Transport in Cubic Semiconductors Si, Ge, AIAs and AIP: Scattering Channels and Size Effects", *Nano Ex.* 5, 035018 (2024).

Poster #6: Self-Consistent Spectra of the Strongly Correlated Bose-Fermi Gas**Authors:** Julius Tirpitz**Affiliation:** Heidelberg University

Abstract: We present fully self-consistent spectral functions of a strongly correlated Bose-Fermi mixture near the critical temperature for Bose-Einstein condensation. Our approach employs the Keldysh real-time formalism within the two-particle irreducible effective action, numerically solving Dyson equations for dressed propagators and providing direct access to real-frequency spectra without analytical continuation. Our results reveal qualitative features in the spectral functions that are inaccessible in non-self-consistent treatments, underscoring the importance of self-consistency for accurately capturing dynamical properties in strongly interacting regimes. In addition, we find region of thermodynamic instability that is attributed to an effective, attractive boson-boson interaction mediated by the fermionic component.

Poster #7: Benchmark study for the prediction of band alignment at hetero-interfaces**Authors:** Jean Goossaert**Affiliation:** Université de Rennes

Abstract: A key property for the efficiency of all photovoltaic technologies is the collection of photo-generated charge carriers at the junction between an absorber material and transport layers. This collection is made possible by a proper alignment of the electronic bands at the interface. Evaluating this offset with precision is thus crucial for predicting the cell efficiency. However, most computational techniques fail at reliably predicting valence and conduction band offsets, while sizable discrepancies exist between experimental values as well. Therefore, a benchmark study of the band alignment in various types of heterojunctions is needed. The approach presented in this poster starts from the simplest model junction, the asymmetric Hubbard dimer, and studies the range of validity of several approximations of many-body perturbation theory, in particular GW and GW. The great advantage of this exactly solvable model is to provide a benchmark that, as a function of its parameters, is representative for a wide range of materials.

Poster #8: Layered Multiple Scattering Approach to Hard X-ray Photoelectron Diffraction: Theory and Application

Authors: Trung-Phuc Vo

Affiliation: University of West Bohemia

Abstract: Photoelectron diffraction (PED) is a powerful technique for resolving surface structures with sub-angstrom precision. At high photon energies, angle-resolved photoemission spectroscopy (ARPES) reveals PED effects, often challenged by small cross-sections, momentum transfer, and phonon scattering. X-ray PED (XPD) is not only an advantageous approach but also exhibits unexpected effects. We present a PED implementation for the spin-polarized relativistic Korringa-Kohn-Rostoker (SPRKKR) package to disentangle them, employing multiple scattering theory and a one-step photoemission model. Unlike conventional real-space approaches, our method uses a k-space formulation via the layer KKR method, offering efficient and accurate calculations across a wide energy range (20 8000 eV) without angular momentum or cluster size convergence issues. Additionally, the alloy analogy model enables simulations of finite-temperature XPD and effects in soft/hard X-ray ARPES. Applications include modeling circular dichroism in angular distributions (CDAD) in core-level photoemission of W(110), Si(100) and Ge(100) 3p, excited by circular polarization.

Poster #9: Robust Approximations for the Polarizability of Complex Materials with Applications to Layered Perovskites

Authors: Ilayda Ashgar

Affiliation: École Polytechnique, Laboratoire des Solides Irradiés, Palaiseau, France

Abstract: The aim of this work is to develop computationally efficient approximations for the dielectric function ϵ , and so the polarizability χ of a material. Our approach is based on the closure relations for cases where the conduction states complete the Hilbert space in order to reduce the virtually infinite number of unoccupied conduction bands which will allow us to study bigger systems. I will present the application of this approach to calculate the static dielectric constant of the Silicon crystal and 2D perovskites.

Poster #10: Molecular Insights into the Hydration Mechanism of Kaolinite Surfaces via Machine Learning Force Field

Authors: Halima Said (1) , David Dell'Angelo (1) , Juliette Lainé (2) , Yann Foucaud (3) , and Michael Badawi (1)

Affiliation: (1) L2CM, CNRS et Université de Lorraine (2) ArcelorMittal Global R&D (3) Geo-Ressources, CNRS et Université de Lorraine

Abstract: Kaolinite ($\text{Al}_2\text{Si}_2\text{O}_5(\text{OH})_4$), a naturally abundant clay mineral formed from the alteration of alumina-rich rocks [1,2], plays an essential role in mineral beneficiation processes such as froth flotation, where the surface wettability strongly influences separation efficiency. Understanding how water interacts with kaolinite at the molecular scale is therefore crucial for elucidating its physicochemical behavior. In this study, ab initio molecular dynamics (AIMD) simulations combined with machine learning (ML)-based potential models were employed to investigate the adsorption and structuring of water molecules on kaolinite surfaces. The ML potential was trained to reproduce AIMD reference data, achieving excellent agreement in energy and force predictions, as well as in the computed hydration enthalpy. The ML-accelerated simulations allowed the exploration of larger systems and longer timescales, revealing a realistic hydration film with distinct layering and a well-defined minimum between the first and second water layers. Thermodynamical findings are consistent with previous studies, confirming the validity of our hydrated model [4,5]. These results provide molecular-level insights into the hydration mechanism of kaolinite and validate the use of ML-based force fields as an efficient and accurate approach to study interfacial phenomena relevant to mineral flotation.

References:

- [1] Johnston, C. J.; Pepper, R. A.; Martens, W. N.; Couperthwaite, S.; Miner. Eng. 2022, 176, 107346
- [2] Nnanwube, I. A.; Keke, M.; Onukwuli, O. D.; Clean. Chem. Eng. 2022, 2, 100022
- [3] Tunega, D.; Gerzabek, M.H.; Lischka, H.; J. Phys. Chem. B, 2004, 108, 5930
- [4] Chen, J. ; Min, F. ; Liu, L. ; Lui, C ; Applied Surface Science, 2019, 476, 6

Poster #11: Multiple Strain-Induced Topological Phase Transitions in 1D Polyacene Polymers: A First-Principles Study

Authors: Reza Mosaferi

Affiliation: Insp - Institut Des Nanosciences De Paris - Cnrs - Sorbonne University

Abstract: We investigate how mechanical strain modulates the electronic and optical properties of doubly bridged polyacene polymers using first-principles GW–BSE simulations. Our previous work (Phys. Rev. Materials 9, 044204 – 2025) revealed multiple strain-induced topological phase transitions, associated with aromatic–quinonoid structural rearrangements and band-gap reopenings. Building on this, we show that these topological transitions strongly influence excitonic and optical behavior. Strain reshapes both the quasiparticle and excitonic landscapes, leading to distinct changes in exciton localization and optical absorption. Notably, non-trivial topological phases exhibit enhanced light–matter coupling compared to trivial ones. These findings demonstrate that mechanical strain and topological order act as coupled design parameters, enabling precise control of excitonic interactions and optical responses in flexible π -conjugated polymers for next-generation optoelectronic materials.

Poster #12: Explicit electronic pair correlation in atomic orbital based Jastrow factors

Authors: Andronikos Leventis

Affiliation: University of Luxembourg

Abstract: The quality and accuracy of observables computed using Quantum Monte Carlo methods greatly depend on the choice of appropriately parametrized wave function Ansätze. The simplest Ansatz employed in molecular systems is that of a single Slater determinant modulated by a symmetric Jastrow factor, which is usually limited at two-electron terms. In this work we adapt an orbital-based three/four body Jastrow introduced in refs. [1,2] to include explicit dependence between electronic pair distances. We benchmark different correlation function forms according to total energy, size-consistency and redundancy of parameters, considering atomic species and van der Waals dimers. Furthermore, we distinguish between the importance of the contribution arising from the angular dependency of the atomic Jastrow - expanded in a basis set of Gaussian type functions and polynomials - and the explicit pair correlation function [3].

References:

[1] M. Casula, C. Attaccalite, and S. Sorella, Correlated geminal wave function for molecules: An efficient resonating valence bond approach, *The Journal of Chemical Physics* 121, 7110 (2004).

[2] M. Marchi, S. Azadi, M. Casula, and S. Sorella, Resonating valence bond wave function with molecular orbitals: Application to first-row molecules, *J. Chem. Phys.* 131, 154116 (2009).

[3] P. López Ríos, P. Seth, N. D. Drummond, and R. J. Needs, Framework for constructing generic Jastrow correlation factors, *Phys. Rev. E* 86, 036703 (2012).

Poster #13: Theory of Angle-Resolved Photoemission Spectroscopy of Altermagnetic Mott Insulators

Authors: Lorenzo Lanzini

Affiliation: École Polytechnique , Palaiseau, France

Abstract: Altermagnetism has emerged as an unconventional form of collinear magnetism with spatial rotational symmetries, that give rise to strongly spin-split bands despite of an underlying fully-compensated antiferromagnetic order. Here, we develop a theory for the Angle Resolved Photoemission Spectroscopy (ARPES) response of altermagnetic Mott insulators. Crucially, the spectrum does not simply reflect the non-interacting band structure, but instead a magnetic polaron is formed at low energies, that can be interpreted as a spinon-holon bound state. We develop a spinon-holon parton theory and predict a renormalized bandwidth that we confirm by tensor network simulations. We analyze the characteristic spin-split spectrum and identify a spin-dependent spectral weight of the magnetic polaron, resulting from the altermagnetic symmetry. Our work paves the way for a systematic study of doping effects and correlation phenomena in altermagnetic Mott insulators.

Poster #14: Designing explicit functionals of the potential for the charge density

Authors: Muhammed Hüseyin Gunes (1,2), Vitaly Gorelov (1,2), Matteo Gatti (1,2,3), Lucia Reining (1,2)

Affiliation: (1) LSI, CNRS, CEA/DRF/IRAMIS, École Polytechnique, Institut Polytechnique de Paris, F-91120 Palaiseau, France, (2) European Theoretical Spectroscopy Facility (ETSF), (3) Synchrotron SOLEIL, L'Orme des Merisiers, Saint-Aubin, BP 48, F-91192 Gif-sur-Yvette, France

Abstract: We develop a systematic framework to calculate the charge density as an explicit functional of the Kohn-Sham potential by reusing tabulated results from model systems, particularly the non-interacting homogeneous electron gas. Starting from a Taylor-like expansion in the potential, we construct the Local Potential Approximation (LPA)—analogous to LDA—and include first-order corrections via the Lindhard response. We then use Connector Theory (COT) to simulate higher-order effects without explicitly computing them. COT bridges model and real systems. Our methods yield a series of systematically improving approximations with promising results for charge densities in inhomogeneous systems like cubic helium, without the solving a Schrödinger equation. This work illustrates how model-based expansions provide a scalable path toward constructing functionals of the potential. Finally, we discuss how an analogous approach can yield the interacting charge density as explicit functional of the external potential, by using quantum Monte Carlo data for the interacting homogeneous electron gas.

Poster #15: Spin-polaron fingerprints in the optical conductivity of iridates

Authors: Francesco Cassol,^{1,2}, Leo Gaspard,^{3,1} Cyril Martins,³ Michele Casula,¹ and Benjamin Lenz¹

Affiliation:

1. Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC) Sorbonne Université, CNRS, Paris, France
2. Centre de Physique Théorique (CPHT), Ecole Polytechnique, Institut Polytechnique de Paris, CNRS, Palaiseau, France
3. Laboratoire de Chimie et Physique Quantiques (LCPQ), Université Toulouse III-Paul Sabatier, CNRS, Toulouse, France

Abstract: Since the discovery of their exotic spin-orbital entangled insulating ground state, Ba_2IrO_4 and Sr_2IrO_4 have attracted considerable attention. Their low-energy electronic structure is usually described in terms of the so-called j_{eff} states, and their optical transport spectra are characterized by a peculiar double-peak structure. The two peaks, α and β , are conventionally attributed to excitations within the $j_{eff} = 1/2$ manifold and from the $j_{eff} = 3/2$ to the $j_{eff} = 1/2$ states, respectively. In this work, we employ different numerical techniques to revisit this topic. We compare our simulations with the existing experiments, and we propose an alternative interpretation of the optical conductivity lineshape, based on the presence of spin-polaron quasiparticles within the j_{eff} bands. We calculate the optical conductivity of both compounds within the dynamical mean-field theory of correlated electrons. We show that both α and β peaks display mixed orbital character, in contrast with the conventional interpretation. Subsequently, we calculate the spin-polaron spectral function via the self-consistent Born approximation. By this means, we demonstrate the polaronic nature of the low-energy features of the eigenspectrum and unveil the importance of these quasiparticles in shaping the absorption spectra.

Poster #16: Computational Screening on the Use of Nitride MXene-Supported Single Atom Catalyst for the Hydrogen Evolution Reaction

Authors: Jean Carlos Villa Arpi

Affiliation: Technische Universität Wien

Abstract: Given the growing global energy crisis in recent decades, the search for efficient and sustainable sources and strategies has become increasingly urgent. In recent years, hydrogen production powered by renewable energy has emerged as a promising solution for replacing fossil fuels. However, efficient and cost-effective catalysts are essential to improve performance at all stages of hydrogen generation. In this context, two-dimensional Transition Metal (TM) carbides, nitrides, and carbonitrides (MXenes) have demonstrated significant potential in electrocatalysis, specifically for the Hydrogen Evolution Reaction (HER). Nitride-based MXenes are particularly attractive due to their high electrical conductivity and surface reactivity, making them ideal support platforms for catalyst design. Furthermore, the incorporation of Single Atom Catalysts (SACs) onto MXene surfaces has been recognized as an effective strategy for improving HER activity, constituting a case of self-supported TM based electrocatalyst. Herein, Density Functional Theory (DFT) calculations are employed to investigate HER performance on nitride MXenes-supported SACs structures. MXenes with general formula $M_{n+1}N_n$ ($M = \text{Ti, V, Cr, Zr, Nb, Mo, Hf, Ta, and W}$; $n = \text{number of atomic layers}$) are used as substrates to adsorb single atoms from the 3d, 4d, and 5d transition series, which will be the active site to assess the Volmer step for HER in acidic conditions. This systematic analysis reveals clear relationships between structure and electrocatalytic performance, highlighting $\text{Fe@W}_3\text{N}_2$, $\text{Ru@Mo}_3\text{N}_2$, $\text{Ta@Mo}_3\text{N}_2$, and $\text{Co@Mo}_3\text{N}_2$ systems as promising electroanalytical candidates. These systems exhibit hydrogen adsorption free energies ($\Delta G_{H^*} - \Delta G_{H^*Pt(111)}$) close to 0 eV, framing them as potential structures for experimental designs.

Poster #17: Properties of the Density Matrix for Metavalent Solids**Authors:** Niklas Penner**Affiliation:** RWTH Aachen University

Abstract: In the experimental investigation of phase change materials and their special properties, peculiarities in the bonding character were determined. A corresponding classification of these metavalent materials has so far been carried out on the basis of shared and transferred electrons. The corresponding values were determined using density functional theory (DFT) calculations. Density functional theory has become one of the most universal methods in condensed matter physics and material science to determine and investigate properties of materials. The longer-term goal of the present work is to investigate to which extent the spatial extension of the density matrix is characteristic for the metavalent materials, and whether numerical calculations based on the Kohn-Sham formulation of Density Functional Theory can capture this aspect.

Poster #18: Siesta deployment status across EuroHPC centers and Fugaku

Authors: Anthoni Alcaraz[1], Federico Pedron[1], Jose M. Escartín[1], Pablo Ordejón[1], Alberto García[2]

Affiliation:

[1] ICN2 (CSIC-BIST), Barcelona (Spain)

[2] ICMAB-CSIC, Barcelona (Spain)

Abstract: Siesta has been successfully deployed at eight European computing centers and on Fugaku, demonstrating its portability by being installed on all available architectures: x86, A64FX, and GPU. To facilitate its use, it can be compiled with recipes for cmake, spack, and easybuild, and versions 5.2.2 to 5.4.0 are already available in the EESSI stack. The code is now operational at EUROHPC centers such as Vega, Karolina, and Deucalion, and at those where EESSI is partially integrated, like MareNostrum 5, where its performance and scalability are key for the efficient simulation of large-scale systems.

Acknowledgements: Funded by the Hanami (Hpc AlliaNce for Applications and supercoMputing Innovation: the Europe-Japan collaboration) project via the European High Performance Computing Joint Undertaking (EuroHPC JU) under the European Union's Horizon Europe framework program for research and innovation and Grant Agreement No. 101136269.

Poster #19: Stabilization of sliding ferroelectricity through exciton condensation**Authors:** Matteo D'Alessio [1,2], Daniele Varsano [2], Elisa Molinari [1,2], Massimo Rontani [2]**Affiliation:**

[1] University of Modena e Reggio Emilia, Modena (Italy)

[2] CNR Nanoscience Institute, Modena (Italy)

Abstract: Sliding ferroelectricity is a phenomenon that arises from the insurgence of spontaneous electronic polarization perpendicular to the layers of two-dimensional (2D) systems upon the relative sliding of the atomic layer constituents. Because of the weak van der Waals (vdW) interactions between layers, sliding and the associated symmetry breaking can occur at low energy cost in materials such as transition-metal dichalcogenides. Here we discuss theoretically the origin and quantitative understanding of the phenomenon by focusing on a prototype structure, the WTe_2 bilayer, where sliding ferroelectricity was first experimentally observed. We show that excitonic effects induce relevant energy band renormalizations in the ground state, and exciton condensation contributes significantly to stabilizing ferroelectricity upon sliding beyond previous predictions. Enhanced excitonic effects in 2D and vdW sliding are general phenomena that point to sliding ferroelectricity as relevant for a broad class of important materials, where the intrinsic electric dipole can couple with other quantum phenomena and, in turn, an external electric field can control the quantum phases through ferroelectricity in unexplored ways.

References:

Matteo D'Alessio, Daniele Varsano, Elisa Molinari and Massimo Rontani, "Stabilization of sliding ferroelectricity through exciton condensation", arXiv:2510.01465 (2025).

Acknowledgements: This work was supported in part by: the MaX – MAterials design at the eXascale – European Centre of Excellence, co-funded by the EuroHPC JU and Ministero delle Imprese e del Made in Italy (grant agreement No. 101093374); ICSC – Centro Nazionale di Ricerca in High Performance Computing, Big Data and Quantum Computing – funded by the European Union through the Italian Ministry of University and Research under PNRR M4C2I1.4 (grant CN00000013).

Workshop Presentation Abstracts

Large-scale DFT calculations on nano-scale metallic materials

Speaker: Ayako Nakata

Affiliation: NIMS, Tsukuba, Japan

Abstract: To appropriately describe complex nanoscale structures, such as interfaces, defect complexes, and disordered systems, structural models comprising several thousand atoms or more are often required. To treat these large systems by first-principles method, we have developed a large-scale DFT code CONQUEST [1]. CONQUEST handles large systems by using local orbital support functions to express density matrices, and the computational cost scales cubically to the number of the support functions. Therefore, to reduce the number of support functions without losing accuracy, we have introduced multi-site support functions (MSSF). MSSFs are the linear combinations of pseudo-atomic orbitals from a target atom and its neighbor atoms in a cutoff region. MSSFs correspond to local molecular orbitals so that the number of required support functions can be the minimal. In this study, using MSSFs, we investigate the size and site dependences of atomic and electronic structures in metallic nanoparticles (NPs). We optimized the structures of the NPs with diameters ranging from 0.5 nm to 5.5 nm. It was found that the electronic structure becomes metallic when particle sizes become larger than about 2 nm. Clear site dependence in electronic structure was found in large NPs, particularly for atoms located at the vertex and in the (111) face. To analyze substantial data calculated for large systems efficiently, we propose a method for quantitatively and systematically comparing differences in local electronic structures in large systems by statistical analysis [2].

References:

- [1] A. Nakata, J. S. Baker, S. Y. Mujahed, et al., J. Chem. Phys. 152, 164112 (2020). [0pt] [2] S. Li, T. Miyazaki, A. Nakata, Phys. Chem. Chem. Phys., 26, 20251 (2024).

Excitations in Large Systems using Transition-Based Constrained Density Functional Theory

Speaker: Laura Ratcliff

Affiliation: University of Bristol, UK

Abstract: The ability to accurately predict excited state energies is crucial for investigating molecules and materials, both from a fundamental and applied perspective. For example, thermally activated delayed fluorescence (TADF) has recently proven to be a promising mechanism, which can be exploited for efficient and environmentally friendly organic LEDs. One of the key parameters required for TADF is a small singlet-triplet splitting, making it an important property for investigating and designing new emitters. However, this is complicated by the fact that such excitations may be a combination of both local and charge transfer character, while also being influenced by both internal disorder and the surrounding environment, posing a significant challenge for existing excited state methods. This has motivated the development of a new method, named transition-based constrained DFT (T-CDFT), wherein a constraint is imposed between orbitals, rather than a region of space. This allows the treatment of both local excitations and charge transfer states at a computational cost similar to ground state calculations. T-CDFT has been implemented in the linear-scaling BigDFT code, thereby providing a framework for including explicit environmental and statistical effects on excited state calculations of disordered supramolecular materials, including those used in TADF-based OLEDs.

Electron-phonon coupling at interfaces and grain boundaries from first principles calculations

Speaker: Miguel Pruneda

Affiliation: CINN-CSIC, Oviedo, Spain

Abstract: Electron-phonon coupling plays a crucial role in determining electronic properties at material interfaces, yet computational studies of these interactions in realistic heterostructures remains challenging. Conventional methods based on Density Functional Perturbation Theory combined with Wannier interpolation schemes become computationally prohibitive for large systems containing hundreds of atoms, severely limiting investigations of interfacial phenomena where quantum confinement and symmetry breaking drive novel electronic phases, such in oxide heterostructures that sustain 2DEG with superconducting properties, or at grain boundaries of semiconductors, which might hold localized defect states that affect thermal, electronic, and optoelectronic properties. We developed a computational approach based on finite differences and localized basis orbitals to calculate electron-phonon coupling in these complex systems. This methodology operates at computational costs comparable to standard phonon dispersion calculations with finite differences, maintaining full compatibility with localized basis set frameworks. The technique enables systematic studies of electron-phonon interactions across diverse material interfaces at the nanoscale, including oxide superlattices, grain boundaries, and other low-dimensional defects in solids. I will illustrate the strength of the method by discussing two examples where we identified interfacial phonon modes that couple to confined electronic states: grain boundaries in crystalline silicon, and LaAlO₃/SrTiO₃ interfaces. This computational breakthrough opens new avenues for understanding the microscopic mechanisms underlying emergent phenomena in heterostructures, providing a powerful tool for designing materials with tailored electronic properties through controlled interfacial engineering.

Impact of MxP on Dense Eigenvalue Computation

Speaker: Toshiyuki Imamura

Affiliation: RIKEN-CCS, Kobe, Japan

Abstract: Mixed precision (MxP) has evolved from residual correction iterations, such as the Ozaki scheme-1 for Error-Free Transform (EFT) based compensated decomposition, to Ozaki scheme-2, which employs Chinese Remainder Theory (CRT). This discussion examines the current status of the Ozaki schemes and current applications, focusing on both hardware and software components. These include simple substitution of GEMM routines in eigenvalue solvers, partial mixed-precision operations within traditional eigenvalue algorithms, and the potential advantages of integrating more advanced low-precision operations with “refsyevd,” Ogita-Aishima’s iterative refinement method for eigenvalues.

Expanding ChASE functionalities to solve for the Bether-Salpeter equation for pseudo-Hermitian Hamiltonians

Speaker: Clément Richefort

Affiliation: Julich Supercomputing Centre , Germany

Abstract: Studying the electronic structure of materials requires solving the Bethe-Salpeter Equation through the computation of all or several eigenpairs. Iterative eigensolvers are often preferred for this task since they scale better on massively parallel platforms and tend to leverage the computational power of modern exascale systems. In particular, the ChASE eigensolver permits to compute several thousands of the most extreme eigenpairs of Hermitian matrices with good scalability. This work presents an upgrade of ChASE for the pseudo-hermitian Hamiltonians of materials science, and achieves similar convergence and performance to the Hermitian case. By exploiting structural and spectral properties of the matrix, we upgrade each ingredient of ChASE independently. In particular, we present an oblique variant of Rayleigh-Ritz without explicit construction of the dual basis, and a parallel implementation of the matrix-product operation with limited amount of global communications.

Title TBA

Speaker: Laura Grigori

Affiliation: EPFL, Lausanne, Switzerland

Abstract: TBA

High-throughput Quasiparticle self-consistent GW

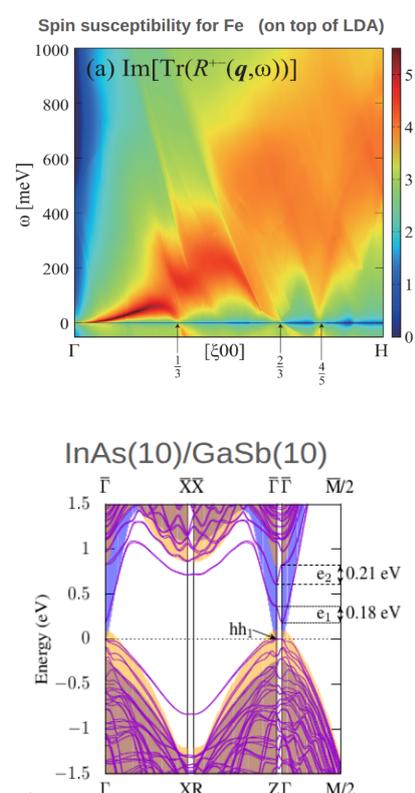
Speaker: Takao Kotani^{1,2}

Affiliation: 1. Advanced Mechanical and Electronic System Research Center, Department of Engineering, Tottori University, Tottori 680-8551, Japan

2. Center for Spintronics Research Network (CSRN), Osaka University, Toyonaka, Osaka 560-0831, Japan

Abstract: Quasiparticle self-consistent GW (QSGW) [1] is one of the best to obtain the one-body Hamiltonian for the independent-particle picture. QSGW requires the self consistency not only for the electron densities but also for the screened Coulomb interactions. After giving the basics of QSGW, I will show two kinds of calculations based on QSGW. One is the spin fluctuations.

We have succeeded to obtain ultra high-resolution map of spin fluctuations. We can interpret it in the generalized Heisenberg model with time-dependent $J(t-t')$ [2]. The other is the multiplet excitations [3], e.g., Cr/Al₂O₃, we obtain model Hamiltonian based on the matching principle with the QSGW results as a reference. This results good agreements with experiments. High High-throughput contains two aspects, robustness and computational speed. For the robustness, we confirmed that we have succeeded to perform automated calculation for 1500 materials taken from the Material Project database [3]. For the speed, we have done GPU implementation of QSGW. This allows us to handle ~ 40 atoms per cell easily. With one node (128 core) with four A100 GPU, we observed 38 times faster computation in our mixed precision implementation than that with four nodes. We have obtained the band structure of quantum well of type-II InAs/GaSb in the right fig.



References:

[1] D. Deguchi et al. (2016), 10.7567/JJAP.55.051201

[2] H. Okumura, K. Sato, T. Kotani (2021), 10.7566/JPSJ.90.094710

[3] H. Saito et al. (2023), Phys. Rev. B 108, 035141, K. Suzuki et al. (2023), Phys. Rev. Res 5, 013111

[4] S. Takano et al. (2025)

<https://arxiv.org/html/2507.19189v1> QSGW database is in <https://ecalj.github.io/ecaljdoc/>

[5] M. Obata, T. Kotani, T. Oda, Computational Materials Science 260, (2025) 114190

Self-consistent random phase approximation and optimized hybrid functionals for solids

Speaker: Maria Hellgren

Affiliation: IMPMC, Sorbonne Université, Paris, France

Abstract: The random phase approximation (RPA) and the GW approximation share the same total energy functional but RPA is defined on a restricted domain of Green's functions generated by a local Kohn-Sham (KS) potential. Here, we show that fully self-consistent RPA KS potentials for solids are feasible by solving the optimized effective potential equation. In addition, we introduce an approach for reliably optimising the fraction of exchange of low-cost hybrid functionals, using the variational minimum of the RPA. The resulting RPA and optimized hybrid potentials are shown to give superior densities, orbitals and eigenvalues as compared to semi-local approximations in DFT, leading to improved structural properties and phonons, as well as more accurate and well-defined starting points for G_0W_0 calculations. Results will be shown for simple solids and more challenging systems, such as TiO_2 and TiSe_2 .

Computing Observables with Quantum Monte Carlo from Excitations to One-Body Reduced Density Matrices

Speaker: Vitaly Gorelov

Affiliation: CNRS - Laboratoire des Solides Irradiés, France

Abstract: This talk will discuss ways to compute observables beyond the ground-state energy with Quantum Monte Carlo (QMC), with the main focus being around the finite-size effects. I'll first cover excited states: for charged (quasiparticle) excitations we obtain gaps from total-energy differences in $N\pm 1$ systems, emphasizing twist averaging and Coulomb finite-size corrections; for neutral excitations we target low-lying states, and discuss a ground-state-only route to neutral gaps and the characteristic ($1/L \rightarrow 1/L^3$) finite-size crossover (see Refs. [1] and [2]). I'll then turn to the one-body reduced density matrix (1RDM) and the electron density as observables that characterize correlation. We benchmark QMC estimators on the helium atom to ask whether better energies imply better observables, identify efficient estimator/optimization strategies [3]. We also show that careful finite-size treatments (twist/boundary-condition averaging, size-consistent estimators, improved Coulomb corrections) enable accurate RDMs in crystalline silicon [4]. These results translate into practical QMC procedures for excitations and RDMs with controlled finite-size behavior.

References:

[1] Y. Yang et al., Phys. Rev. B 101, 085115 (2020)

[2] V. Gorelov et al., Condensed Matter Physics 26, 33701 (2023)

[3] C. Rodriguez Perez, V. Olevano, F. Sottile, V. Gorelov, in preparation (2025)

[4] C. Rodriguez Perez, M. Holzmann, F. Sottile, V. Gorelov, in preparation (2025).

First-Principles Insights into the Opto-Electronic Properties of Novel 2D and Layered Materials

Speaker: Maurizia Palummo

Affiliation: Dipartimento di Fisica Università di Roma Tor Vergata, Italy

Abstract: The advancement of future opto-electronic technologies hinges on the discovery and in-depth understanding of novel low-dimensional materials. Ground and excited-state first-principles simulations provide a powerful framework to uncover the microscopic mechanisms that determine their properties, while offering predictive insights that can guide experimental design. In this talk, I will present results, obtained in the last years, through parameter-free atomistic simulations devoted to the investigation and control of the opto-electronic response of emerging 2D and layered systems. By employing Density Functional Theory (DFT) combined with Many-Body Perturbation Theory (GW and Bethe-Salpeter Equation), we address key aspects such as: (i) band gap renormalization, (ii) strong light–matter interaction, (iii) excitonic effects and radiative lifetimes, and (iv) the impact of doping and chemical substitution as effective tuning strategies. Special focus will be given to material families with promising opto-electronic potential, including Transition Metal Dichalcogenides (TMDs) and 2D/layered halide perovskites. I will also discuss the excitonic properties of MoSiN compounds and carbon-based 2D triangulene polymers, underscoring their relevance for emerging technological applications.

Non-linear response functions from real-time simulations

Speaker: Claudio Attaccalite

Affiliation: CNRS/Aix-Marseille Université, CINaM laboratory, Marseille, France

Abstract: The nonlinear optical responses of both bulk and low-dimensional materials present exciting opportunities for the development of next-generation optoelectronics. To investigate these properties, we have developed an efficient, real-time formalism that enables us to calculate nonlinear responses, including correlation effects such as band gap renormalisation, the local field effects and electron-hole interactions. We have applied this formalism to study various nonlinear optical phenomena, including second/third harmonic generation [1, 2], shift current [3] and sum frequency generation [4]. In this talk, I will introduce the different nonlinear optical response functions, their possible applications and present the formalism used to study them.

References:

- [1] *Nonlinear optics from an ab initio approach by means of the dynamical berry phase: Application to second-and third-harmonic generation in semiconductors.* , C. Attaccalite, , and M. Grüning. *Physical Review B—Condensed Matter and Materials Physics* 88.23 (2013): 235113.
- [2] *Tunable second harmonic generation in 2D materials: comparison of different strategies.*, S. Grillo et al. , *SciPost Physics Core* 7.4 (2024): 081.
- [3] *Shift current in 2D Janus Transition-Metal Dichalcogenides: the role of excitons*, Y. Mao, J. Zhou, M. Grüning, C. Attaccalite, <https://arxiv.org/abs/2506.16067>
- [4] *Sum frequency generation from real-time simulations in two-dimensional crystals*, M. N. Pionteck, et al. , <https://arxiv.org/abs/2503.07095>

Optical absorption in hexagonal-diamond Si and Ge nanowires: insights from STEM-EELS experiments and ab initio theory

Speaker: Michele Amato

Affiliation: LPS, Université Paris-Saclay, France

Abstract: Hexagonal-diamond (2H) group IV semiconductors have emerged as promising materials for next generation silicon-compatible optoelectronics, offering potential pathways toward efficient light emission in group IV platforms [1-3]. Despite growing interest in their electronic structure, a clear experimental understanding of their optical absorption properties remains lacking. In this work, I will present and discuss the first comprehensive investigation of the optical absorption of 2H-Si and 2H-Ge nanowires, combining high-resolution scanning transmission electron microscopy (STEM), monochromated electron energy-loss spectroscopy (EELS), and ab initio simulations [4]. The nanowires were grown in situ within a transmission electron microscope as branches on GaAs stems, enabling exceptional control over structural quality. The resulting nanowires are single crystalline, strain-free, and virtually defect-free, with no detectable substrate contamination, providing a pristine platform for probing their intrinsic dielectric response. Our results reveal a strong enhancement in the visible-range absorption of 2H-Si compared to its cubic (3C) counterpart, with a well-defined absorption onset above 2.5 eV. For 2H-Ge, we observe a low-energy absorption onset near 1 eV, consistent with its reduced bandgap, though no distinct peak is detected at the direct bandgap transition, in line with predictions from first-principles calculations [5]. Additionally, a spectral feature around 2 eV in aloof-beam EELS is attributed to a thin 3C-Ge shell surrounding the nanowires [4]. These findings mark a significant step toward understanding the structure-property relationships in hexagonal group IV nanostructures. They also provide critical insight into the optical behavior of 2H-Si and 2H-Ge, offering guidance for the development of hexagonal-phase-based optoelectronic and photonic devices.

References:

- [1] Fadaly, E. M. et al. Direct-bandgap emission from hexagonal Ge and SiGe alloys. *Nature* 2020, 580, 205–209.
- [2] Amato, M. et al. Crystal phase effects in Si nanowire polytypes and their homojunctions. *Nano Lett.* 2016, 16, 5694–5700.
- [3] Galvão Tizei, L. H. and Amato, M. Electronic structure and optical properties of semiconductor nanowires polytypes. *Eur. Phys. J. B* 2020, 93, 1–20.
- [4] Galvão Tizei, L. et al. Optical Absorption and Dielectric Response of Hexagonal-Diamond Group IV Nanowires. *Nano Lett.* 2025, 25, 8604–8611.
- [5] Rödl, C. et al. Accurate electronic and optical properties of hexagonal germanium for optoelectronic applications. *Phys. Rev. Mater.* 2019, 3, 034602.

Simulating the optical properties of solids using ab-initio BSE: there is more than meets the eye

Speaker: Claudio Quarti

Affiliation: University of Mons, Belgium

Abstract: The ab-initio solution of the Bethe Salpeter Equation (BSE) represents the “golden-reference” for the prediction the optical properties of solids.[1-3] In connection with first a principle GW calculation, this approach accurately describes the electron-hole binding via the knowledge of the non-local screened Coulomb interaction, without assumptions, in striking contrast to methods like range-separated exchange-correlation functionals.[2] As a result, the ab-initio BSE method is able to accurately predict the optical spectrum of solids, providing very good estimates of important quantities, like the exciton binding energy.[3-4] The analysis of the results of ab-initio BSE solutions however seldom goes beyond the bare accordance of the predicted absorption spectrum with the experimental one, leaving a lot of information unexplored.[3-4] Here we show that the ab-initio solution of BSE can provide a unique insight on the optical properties of materials, complementing the experimental characterization. For this purpose, we reference to the study case of 2D halide perovskites, natural quantum well structures characterized by a strong spin orbit interaction, as well as by a spatially inhomogeneous dielectric function. Starting from highly symmetric models, and progressively incorporating realistic details in the atomistic models, we interpret the BSE results on the basis of group-theory expectations and compare them with the experimental findings.[5] In this way, we successfully assign the fine structure of the lowest energy exciton, also resolving a debate on the interpretation of the spectra.[6] In addition, we assign the full Wannier series up to the 4s component and we unveil spin properties of this class of materials. We hope the present study will inspire theoreticians to dig more into the results of their BSE calculations, so to maximize the information from their calculations.

References:

[1] Nat. Natotechnol, 17, 45-52 (2022).

[2] Chem. Soc. Rev., 47, 1022-1043 (2018).

[3] Nano Lett. 23, 8155–8161 (2023).

[4] J. Phys. Chem. Lett. 9, 5891–5896 (2018).

[5] Adv. Opt. Mater., 12, 2202801 (2024).

[6] Sci. Adv. 7, eabk0904 (2021).

Vibronic Pathway Engineering for Efficient Exciton Separation in High-Efficiency Nonfullerene OSCs

Speaker: Azusa Muraoka

Affiliation: Japan Women's University, Japan

Abstract: The sun supplies abundant energy that can be harvested as electricity. Organic solar cells (OSCs) with nonfullerene acceptors (NFAs) are a promising renewable technology, with NFA-based thin-film OSCs already exceeding 20% efficiency. Further improvements require increasing the short-circuit current density (J_{sc}). Exciton dissociation proceeds via two mechanisms: a “hot process” yielding charge-separated (CS) states directly, and a “cool process” via intermediate charge-transfer (CT) states. Vibronic coupling at the donor/acceptor interface determines the dominant pathway, making interfacial exciton dynamics critical for device design [1, 2]. We hypothesize that CT excitons form weakly bound polaron pairs that dissociate via nonadiabatic vibrational coupling without full relaxation. Using TDDFT, we evaluate excited-state properties, electronic structure, electron–hole distance, electronic coupling, and Huang–Rhys factors of PTB7/BTA x ($x = 1, 3$) complexes [3]. PTB7/BTA3, consistent with higher J_{sc} , shows larger CT separation and stronger D \rightarrow A transitions, indicating enhanced charge separation. In contrast, PTB7/BTA1 exhibits higher Huang–Rhys factors from low-frequency modes, implying stronger nonadiabatic relaxation. These results show that tuning vibronic interactions can steer exciton dissociation pathways, providing guidance for high-efficiency OSC design.

References:

[1] H. Imahori, et. al, *Acc. Res.*, 2021, 2, 501-514.

[2] A. Muraoka, et. al, *Phys. Chem. Chem. Phys.*, 2018, 20, 12193-12199. [3]

S. Ikeyama, et. al, *J. Chem. Phys.*, 2023, 159, 044307-1/044307-11.

Next-generation perovskites and inspired energy materials from first-principles.**Speaker:** George Volonakis**Affiliation:** Université de Rennes, France

Abstract: Ab initio simulations have emerged as indispensable tools for probing, modeling, and elucidating the properties of complex materials, like for example, halide perovskites and materials that have been inspired by them. Over the past ten years, these computational approaches have yielded valuable insights into the atomic-level processes that dictate the behavior of these systems. I will share our most recent work on the electronic structure of key halide-based materials including prototypical layered halide perovskites, vacancy-ordered double perovskites, and low-dimensional perovskite analogues. I will emphasize the electronic characteristics that drive their optical responses and shape their experimental performance. Our results show both the potential and the limitations of these materials in diverse optoelectronic technologies, ranging from indoor and outdoor solar cells to light-emitting devices. Concluding the talk, I will discuss our advanced ab initio investigations of charge-carrier transport, contrasting three-dimensional and layered halide perovskites, and introduce a new, parameter-free approach for accurately resolving their electronic structure.

1D and 2D molecular nanoarchitectures: electronic insights from DFT-based simulations

Speaker: Aran Garcia-Lekue

Affiliation: DIPIC (Donostia International Physics Center), Ikerbasque (Basque Foundation for Science), Basque Country, Spain

Abstract: Currently, on-surface synthesis methods allow creating atomically precise 1D and 2D carbon-based nanostructures with identical and homogeneously distributed pores.[1,2] In tandem with the experimental advances, theory and simulation emerge as essential partners in order to achieve an atomic level understanding and control of their properties. In this talk, I will present some studies of porous graphene nanoribbons (GNRs) and nanoporous graphene (NPG), that we have recently performed in our group. Combining density functional theory (DFT) with tight-binding (TB) models and non-equilibrium Green's functions (NEGF) approach, and in collaboration with our experimental colleagues, we have investigated their structural, electronic and transport properties. On the one hand, we have explored porous GNRs containing biphenylene units that merge laterally giving rise to novel porous 2D networks.[3] Further, we have reported on the anisotropic current propagation in NPG, which can be finely tuned either by intrinsic changes in its atomic structure or by stacking it on graphene.[4,5] Interestingly, we have also demonstrated that scanning tunneling microscopy (STM) experiments performed for such porous carbon-based systems often exhibit deceptive electronic confinement effects.[6]

References:

- [1] Qin et al., Commun. Chem. 7, 154 (2024)
- [2] Moreno et al., Commun. Chem. 7, 219 (2024)
- [3] Angulo-Portugal et al., (under review)
- [4] Moreno et al., J. Am. Chem. Soc. 145, 8988 (2023)
- [5] Diaz de Cerio et al., Nano Letters 25, 1281 (2025)
- [6] Piquero-Zulaica et al. 15, 1062 (2024)

First-Principles and Data-Driven Approaches for the Computational Design of Functional Heusler Alloys

Speaker: Terumasa Tadano

Affiliation: NIMS, Tsukuba, Japan

Abstract: Heusler alloys have been extensively studied for their potential applications in various functions, including spintronic devices, shape-memory alloys, and both longitudinal and transverse thermoelectricity. To utilize these alloys effectively, it is often necessary to optimize multiple physical properties simultaneously while ensuring their stability. This task can be challenging due to the vast range of possibilities. In recent years, significant progress has been made in constructing and utilizing material databases generated through first-principles calculations based on density functional theory (DFT). These databases, along with advanced machine-learning (ML) techniques, are expected to aid in the efficient exploration of the extensive chemical space of functional materials. In this presentation, we will discuss our recent activities in database generation and the development of ML models for property prediction [1,2]. First, we will introduce the DXMag Computational HeuslerDB [3], which contains comprehensive properties of approximately 28,000 ternary Heusler alloys computed using DFT. Next, we will present an ML model capable of predicting material properties directly from crystal structures. This model is built by leveraging transfer learning from the state-of-the-art universal ML interatomic potential (uMLIP), eSEN-30M-OAM [4], and its parameters in the final message-passing layers are refined using the HeuslerDB dataset. Our model demonstrates high precision in predicting various properties, including phonon stability, magnetic moments, and magneto-crystalline anisotropy (MCA) energy. By applying the developed ML models to 131,544 quaternary and 104,139 all-d Heusler alloys, we were able to efficiently screen around 1,300 candidates expected to exhibit large MCA energy, specifically $|K1| > 1 \text{ MJ/m}^3$. Subsequent DFT calculations confirmed that approximately 80% of these candidates met this criterion. This work highlights the reliability and efficiency of the developed ML-assisted framework for screening functional materials.

References

- [1] E. Xiao and T. Tadano, *Acta Mater.* 297, 121312 (2025)
- [2] E. Xiao and T. Tadano, arXiv:2508.20556
- [3] <https://www.nims.go.jp/group/spintheory/database/>
- [4] Fu, X. et al. arXiv:2502.12147.

Exploring zero-temperature phase diagrams with neural network quantum states

Speaker: Marcus Holzmann

Affiliation: LPMMC, Université Grenoble-Alpes, France

Abstract: Iterative backflow [1,2] and neural network quantum states [3] provide highly accurate representations of many-body ground state wave functions. Variational Monte Carlo calculations based on neural backflow quantum states can overcome major limitations of quantum Monte Carlo methods, in particular concerning the exploration of zero temperature phase diagrams. I will give an overview over recent results on the electron gas [4], hydrogen [5], and on the liquid-solid transition of two-dimensional helium [6].

References:

- [1] M. Taddei, M. Ruggeri, S. Moroni, and M. Holzmann, Phys. Rev. B 91, 115106 (2015).
- [2] M. Ruggeri, S. Moroni, and M. Holzmann, Phys. Rev. Lett. 120, 205302 (2018).
- [3] G. Carleo and M. Troyer, Science 355, 602 (2017).
- [4] M. Holzmann and S. Moroni, Phys. Rev. Lett. 124, 206404 (2020).
- [5] D. Linteau, S. Moroni, G. Carleo, M. Holzmann, cond-mat/2504.07062.
- [6] D. Linteau, G. Pescia, J. Nys, G. Carleo, and M. Holzmann, Phys. Rev. Lett 134, 246001 (2025).

Modelling electrolytes for energy storage applications via machine learning-based simulations

Speaker: Alessandra Serva

Affiliation: PHENIX Laboratory, Sorbonne University, CNRS, France

Abstract: In energy storage (e.g., supercapacitors and batteries) and catalysis applications, the electrolyte is one of the key components influencing efficiency. Gaining an atomistic understanding of the composition-property relationship is therefore essential for the rational design of new electrolytes with improved performances. Molecular dynamics (MD) simulations have proven to be a powerful tool for providing such microscopic insight. In particular, in recent years, machine learning potentials have shown to be promising for modeling complex electrolytes, especially in cases where classical potentials fail to capture essential structural and thermodynamic properties. In this talk, I will present two examples of electrolytes investigations using machine learning-based simulations: (i) a protic ionic liquid, a promising material notable for its ability to decouple proton transport from ion diffusion, to model the proton transfer mechanism; and (ii) sodium metal halides and sodium metal oxyhalides for solid-state sodium-ion batteries, to unravel the relationship between structure, conductivity and transport mechanisms.

Simulation, theory, and machine learning approaches for investigating materials and molecular systems.

Speaker: Tomomi Shimazaki

Affiliation: Graduate School of Nanobioscience, Yokohama City University, 22-2, Seto, Kanazawa, Yokohama, 236-0026, Japan

Abstract: This presentation explores research on materials and molecules through simulation, theory, and machine learning. In the simulation section, we focus on perovskite solar cell materials, which have gained attention in recent years due to their high power conversion efficiency (PCE). While lead (Pb) is commonly used in these devices, its toxicity has prompted interest in lead-free tin (Sn)-based perovskites. However, Sn-based perovskites are prone to forming defect states on the surface, which hinder the achievement of high PCE. To address this issue, molecular passivation processes have been introduced in device fabrication. We investigate the molecular-level mechanisms of these processes using first-principles simulations.[1-3] In the theory section, we discuss the dielectric-dependent density functional theory (DFT) method.[4- 5] This approach exhibits system-dependent characteristics, where the form of the exchange- correlation functional varies according to the target material or molecule. In particular, the fraction of Hartree-Fock exchange is proportional to the inverse of the dielectric constant. This method has recently been extended from inorganic materials to molecular systems, and we will examine its theoretical foundations. Finally, in the machine learning section, we present an analysis of radical reactions involved in the synthesis of acrylic polymers. Using reaction data, we apply theoretical and machine learning techniques to extract insights, with a particular focus on the machine learning methods used for data analysis,[6] especially the (modified) convex clustering regression approach.

References:

- [1] E. Kino, M. Takagi, M. Tachikawa, Y. Yamashita, and T. Shimazaki, *J. Chem. Phys.*, 2025, 163, 104703.
- [2] E. Kino, M. Takagi, T. Naito, M. Tachikawa, Y. Yamashita, and T. Shimazaki, *Phys. Chem. Chem. Phys.*, 2025, 27, 7429.
- [3] T. Naito, M. Takagi, M. Tachikawa, K. Yamashita, and T. Shimazaki, *J. Phys. Chem. Lett.*, 2023, 14, 6695.
- [4] T. Shimazaki and M. Tachikawa, *Phys. Chem. Chem. Phys.*, 23, 21078, 2021
- [5] T. Shimazaki and M. Tachikawa, *J. Chem. Phys.*, 161, 014107, 2024.
- [6] M. Takagi, T. Shimazaki, O. Kobayashi, T. Ishimoto, M. Tachikawa, *Phys. Chem. Chem. Phys.*, 27, 1772, 2024.

Effective interactions in many-body perturbation theory

Speaker: Lucia Reining

Affiliation: LSI, Ecole Polytechnique Palaiseau, CNRS, France

Abstract: Many-body perturbation theory is usually formulated in terms of a screened, instead of the bare Coulomb interaction. There is, however, no unique prescription for what this screened interaction should be. This is one of the reasons for the many different flavors that can be found in ab initio calculations, for example, for Hedin's GW approximation [1] for the self-energy. In this talk we will analyze the situation and give arguments for certain choices, both for the calculation of spectroscopic quantities and for the total energy. These choices can be formulated in terms of approximate vertex corrections to the GW expression, where W is defined to be the exact test charge-test charge screened interaction [2]. We then broaden the concept of the screened interaction to a generalized effective interaction, for which we derive in principle exact equations as well as promising approximations. We show that this allows one to go beyond the GW approximation in an efficient way, avoiding the computational complexity of full vertex corrections. Further arguments based on a model self-energy will be added. Illustrations include quasiparticle energies, full spectral functions and total energies for model systems and real materials.

References:

[1] Lars Hedin, Phys. Rev. 139, A796 (1965)

[2] Abdallah El Sahili, Francesco Sottile and Lucia Reining, Journal of Chemical Theory and Computation 20, 1972 (2024)

Efficient many-body perturbation theory calculations of (doped) 2D materials: Applications to ARPES and EELS spectroscopies

Speaker: Andrea Ferretti

Affiliation: CNR, Istituto Nanoscienze, Modena, Italy

Abstract: Many-body perturbation theory methods are able to accurately predict quasiparticle (QP) and spectroscopic properties of several classes of materials. However, the calculation of the QP band structure of 2D materials is known to require a very dense BZ sampling. For 2D semiconductors, large q-point grids are required to describe the sharp q-dependence of the dielectric matrix in the long-wavelength limit ($q \rightarrow 0$). Moreover, intraband contributions need to be included when dealing with metals. In this talk, I will first describe a new methodology able to significantly improve the convergence of the QP corrections in 2D semiconductors with respect to the BZ sampling by combining a Monte Carlo integration method with an interpolation scheme able to describe the sharp dispersion of the dielectric function. Then, I will show how to extend the approach to treat metals and how to integrate the new methodology with a multi-pole expansion of the frequency dependence of the screening, able to reach the accuracy of full-frequency methods with a coarse sampling of the frequency space. This combined approach has been used to obtain accurate results for doped graphene and MoS₂ QP band structures. Additionally, we have also addressed the simulation of electron energy loss spectra (EELS) of pristine and doped graphene, using both RPA and BSE response, showing excellent agreement with recent high-resolution experimental data.

Green's function approaches to the spectroscopy in photovoltaic organic molecules and photosynthesis chlorophyll A and B in LHC II

Speaker: Valerio Olevano

Affiliation: CNRS and Univ. Grenoble Alpes, France

Abstract: The absorption of light and the ensuing electronic excitations constitute the primary step for solar energy conversion in both photovoltaic and photosynthesis. Yet, the understanding and a predictive theoretical description of these processes remains a grand challenge. Progress in this direction carries the promise of not only enhancing photovoltaic performance, but also move us closer to the realization of the long-sought dream of artificial photosynthesis as a scalable route to clean energy. In this talk we present an ab initio many-body Green's function framework for unraveling excitations and spectroscopy in both photovoltaic and photosynthetic complexes. We first validate the methodology (e.g. the Bethe-Salpeter equation) and the approximations (e.g. GW) through benchmark comparisons against exact solutions for prototypical systems, such as helium [1,2] and the hydrogen molecule [3], thereby establishing a solid foundation for its predictive power. We then demonstrate applications to the ionization potentials and gaps in organic photovoltaic molecules [4] and DNA/RNA nucleobases [5], followed by a detailed analysis of photoabsorption spectra and the excitonic structure in chlorophyll A and B in their in vivo conformations within the light-harvesting complex (LHC) II [6]. In particular, we reveal how subtle charge-transfer differences on the Soret band and Q excitons, underpin the unique capability of chlorophyll A to drive photosynthesis, in contrast to the purely light-harvesting role of chlorophyll B.

References:

- [1] J. Li, M. Holzmann, I. Duchemin, X. Blase and V. Olevano, "Helium atom excitations by the GW and Bethe-Salpeter many-body formalism", *Phys. Rev. Lett.* 118, 163001 (2017).
- [2] J. Li, N. D. Drummond, P. Schuck and V. Olevano, "Comparing many-body approaches against the helium atom exact solution", *SciPost Phys.* 6, 040 (2019).
- [3] J. Li and V. Olevano, "Hydrogen-molecule spectrum by the many-body GW approximation and the Bethe-Salpeter equation", *Phys. Rev. A*, 103, 012809 (2021).
- [4] X. Blase, C. Attaccalite and V. Olevano, "First-principles GW calculations for fullerenes, porphyrins, phtalocyanine, and other molecules of interest for organic photovoltaic applications", *Phys. Rev. B* 83, 115103 (2011).
- [5] C. Faber, C. Attaccalite, V. Olevano, E. Runge and X. Blase, "First-principles GW calculations for DNA and RNA nucleobases", *Phys. Rev. B* 83, 115123 (2011).
- [6] J. Li and V. Olevano, "Bethe-Salpeter equation insights into the photo-absorption function and exciton structure of chlorophyll a and b in light-harvesting complex II", *J. Photochem. Photobiol. B - Biology* 232, 112475 (2022).

Green's functions beyond the GW approximation: Still an open challenge

Speaker: Fabien Bruneval

Affiliation: Section de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, France

Abstract: The GW approximation in Green's function theory gives access to rather reliable electronic energies both for materials and molecules. However, for decades, we have been witnessing an active debate about the most effective "vertex corrections" beyond GW. The inability to decide originates from, firstly, the numerous ways to truncate diagrammatic expansions in many-body perturbation theory; secondly, the impressive performance of the GW approximation itself [1]. In this context, we study the G3W2 diagram [2], which is the dynamical version of the second-order screened exchange (SOSEX) diagram. Numerical results on the GW100 benchmark of molecules show how G3W2 improves over SOSEX however without reaching the accuracy of GW. However, the SOSEX and G3W2 diagram violate an exact property: the positive semi-definiteness of the self-energy [3]. We then show how this property can be mathematically enforced with an appropriate selection of diagrams with an improvement of the results on the GW100 benchmark.

References:

[1] Bruneval et al., <https://doi.org/10.3389/fchem.2021.749779> (2021).

[2] Bruneval, Förster, <https://doi.org/10.1021/acs.jctc.4c00090> (2024).

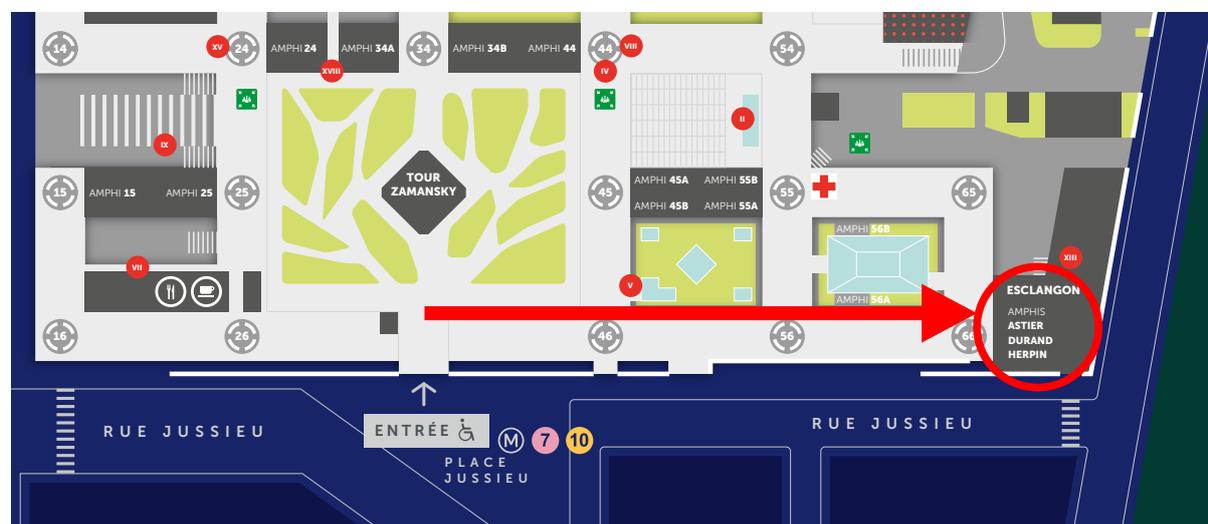
[3] Pavlyukh et al., <https://doi.org/10.1103/PhysRevLett.117.206402> (2016).

Practical information

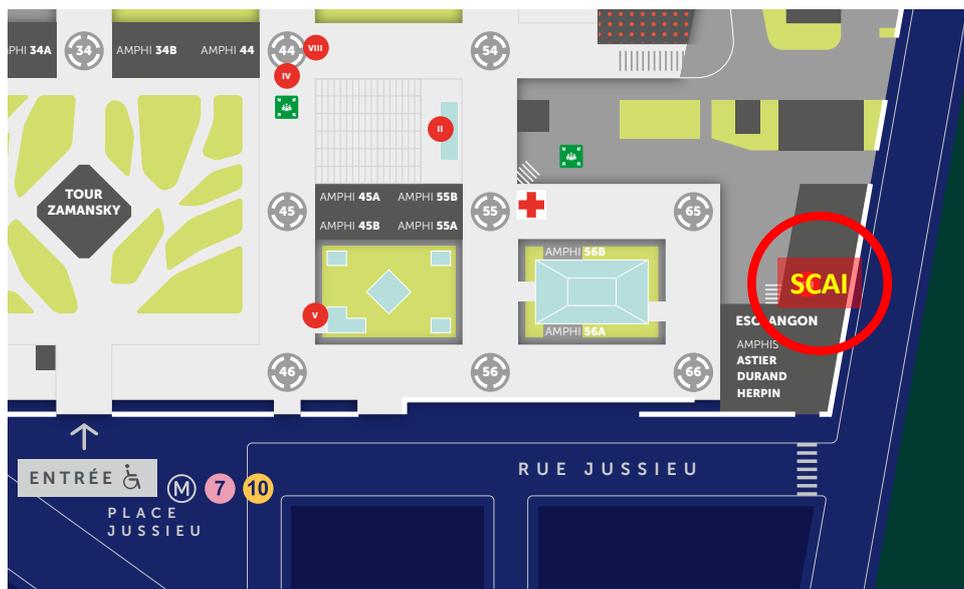
Except for the reception on the boat (bateau-mouche dinner cruise on the Seine), all the other events will take place in the Pierre and Marie Curie campus of Sorbonne University, located at 4 Place Jussieu, in the 5th district of Paris, comfortably reached by metro lines 7 and 10. The main entrance to the campus is situated just in front of the fountain of Jussieu square. Below the full map of the campus.



Below the location of the Durand lecture room (Amphi Durand), reachable from inside the Esclangon building, the main entrance of the room is on the left:



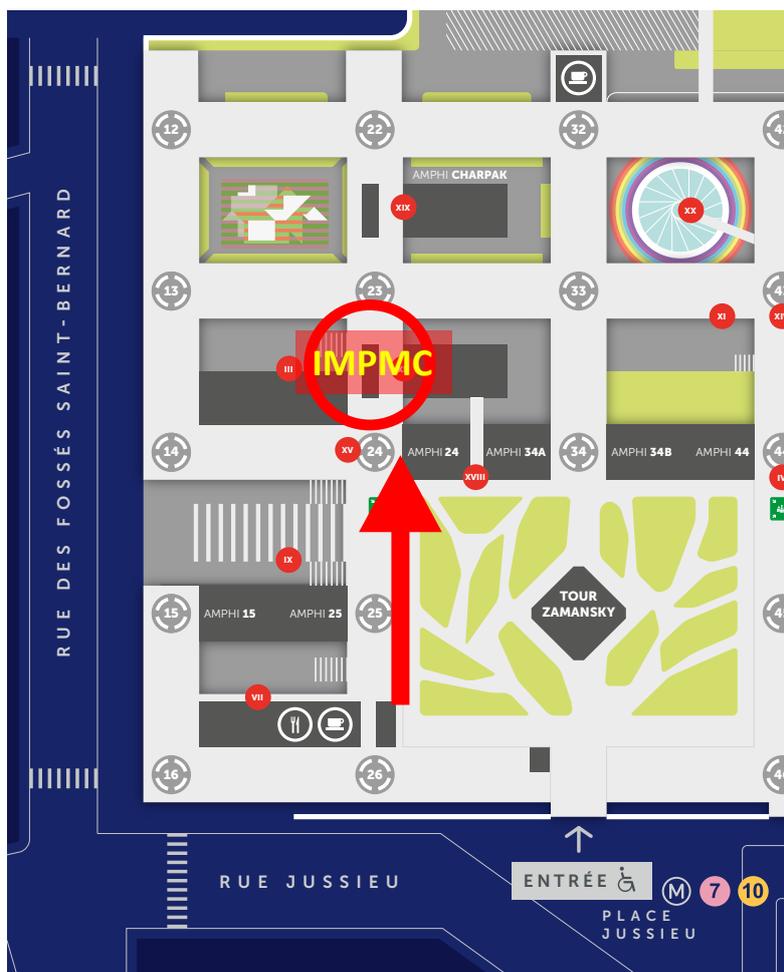
This is the location of the **SCAI** center, accessible by the stairs one can take inside the Esclan-gon building, at the right of the Durand lecture hall, ramping up to the 1st floor:



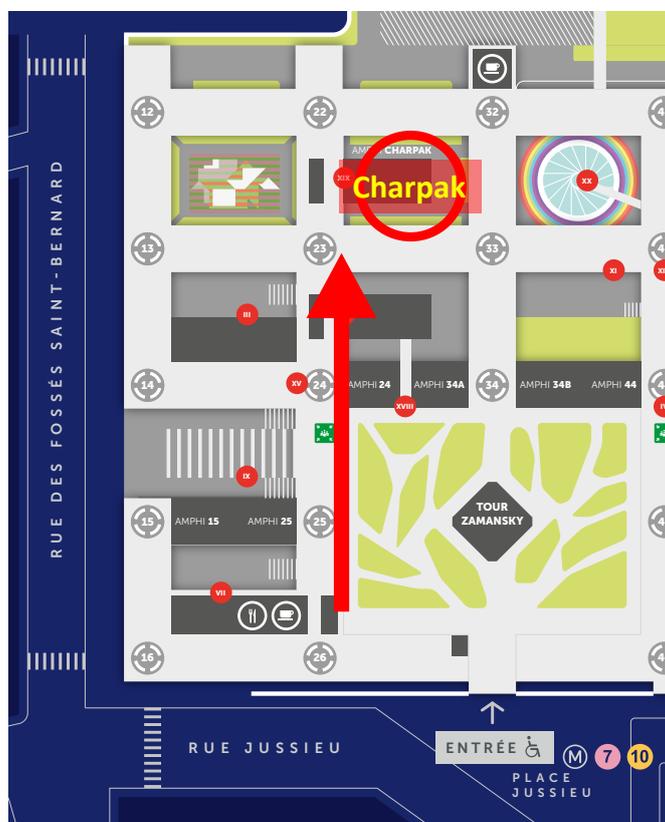
While this is where the Physics Department (**UFR Physique**) is found, accessible by the stairs of Tower 23 (1st floor, corridor 22-23):



Below the position of the conference room of the **IMPMC** institute, accessible from the stairs of Tower 23 (4th floor, corridor 23-24):



The two-day workshop will be held in the Charpak lecture hall (**Amphi Charpak**), accessible from the stairs of Tower 23. From the Jussieu level (the one of the court: “RdJ”), one goes downstairs (basement level: “RdC”), get out of the Tower and walk towards Tower 22. The entrance of the Charpak lecture hall will be on the left:



The dinner cruise flyer by France Tourisme:

VISIT PARIS
TOURS IN FRANCE
CRUISES IN PARIS
PARIS BY NIGHT
SPECIAL EVENTS
SPECIAL

You are here: France Tourisme > Dinner Cruises Paris > Dinner cruise Bistronomique

Dinner cruise Bistronomique, departure from Alexandre III bridge





♥ YOU WILL ENJOY...

- Embark on an **exceptional dinner** in a hushed and musical atmosphere on the Seine
- Enjoy elegant, seasonal cuisine **prepared on board**
- Admire the Eiffel Tower and the treasures of the Capital from the river



Acknowledgements



Funded by
the European Union



This project received funding from the project HANAMI, funded by the **European High Performance Computing Joint Undertaking (EuroHPC JU)** under the **European Union's Horizon Europe framework program** for research and innovation.



This workshop has also been funded by the local **CECAM-FR-MOSER** node of the **European Center for Atomic and Molecular Calculation (CECAM)**, hosted at the Maison de la Simulation in Saclay (Paris area). The node is sponsored by the **Centre national de la recherche scientifique (CNRS)**, the **Commissariat à l'énergie atomique et aux énergies alternatives (CEA)**, the Université Paris-Saclay (UPS), Sorbonne Université (SU), Université Gustav Eiffel (UGE), Ecole Normale Supérieure de Paris (ENS Paris) and Ecole Chimie ParisTech (ENSCP).



We are grateful to **Sorbonne Université (SU)** for hosting the event and for making several Pierre and Marie Curie campus facilities available. We also thank the **SU Physics Department (UFR de Physique)**, for granting the usage of the cluster of personal desktop computers during the skill-building sessions. Finally, we acknowledge the **Sorbonne Cluster for Artificial Intelligence (SCAI)** for hosting some coffee and lunch breaks, offering a nice environment for networking and discussions.

We are indebted with several people who contributed to the realization of this event. In particular, we would like to thank **Ari Paavo Seitsonen (ENS Paris)**, who significantly helped with the preparation of the computer sessions, and **Alain Corriou (SU)**, the system administrator of the computers cluster at the Physics Department.