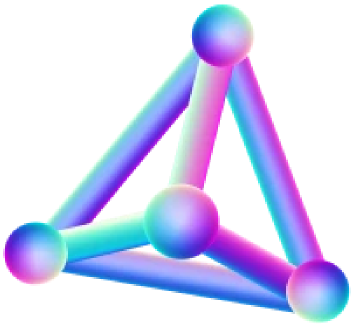

BOOK OF ABSTRACTS

Materials Science from First Principles Workshop

Organizers:

Michele Casula, CNRS and Sorbonne Université, Paris, France
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Edoardo Di Napoli, Forschungszentrum Jülich, Germany
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France Boillod-Cerneux, CEA Fundamental Research Department, Saclay, France

November 5–7

Sorbonne University, Paris, France

Supported by:

HANAMI

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Centre Européen de Calcul Atomique et Moléculaire

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HANAMI-CECAM Materials Science Workshop

Venue and Get-Together dinner cruise: November 5 (Wednesday)

20:45 – 🍷 🚢 **Conference Dinner on the Boat** for all registered participants: Diner croisière Eiffel, boarding at the Alexandre III bridge

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 Palummo** (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*

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

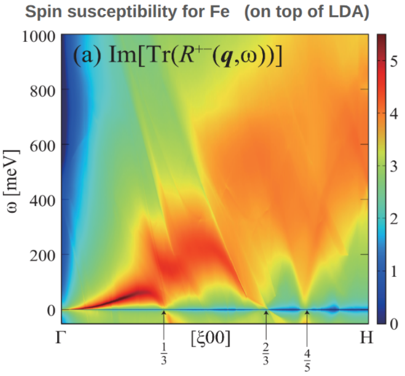
Abstract: TBA

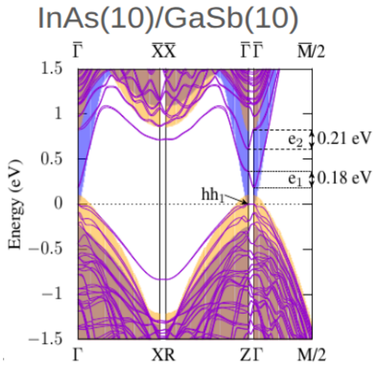
High-throughput Quasiparticle self-consistent GW

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-dependen 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 $\sim$ 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 tyep-II InAs/GaSb in the right fig.


Spin susceptibility for Fe (on top of LDA)


InAs(10)/GaSb(10)

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±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 MoSi N 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 (Jsc). 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/BTAx (x = 1, 3) complexes [3]. PTB7/BTA3, consistent with higher Jsc, shows larger CT separation and stronger D→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: DIPC (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 $|K1| > 1$ 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.

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Exploring zero-temperature phase diagrams with neural network quantum states

Speaker: Marcus Holzmann
Affiliation: LPMMC, Université Greonoble-Alpes, France

Abstract: Iteritive 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:

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[3] G. Carleo and M. Troyer, Science 355, 602 (2017).
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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, Kanazawaku, 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:
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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-wavelegth limit (q -> 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 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:
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[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).
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Green’s functions beyond the GW approximation: Still an open challenge

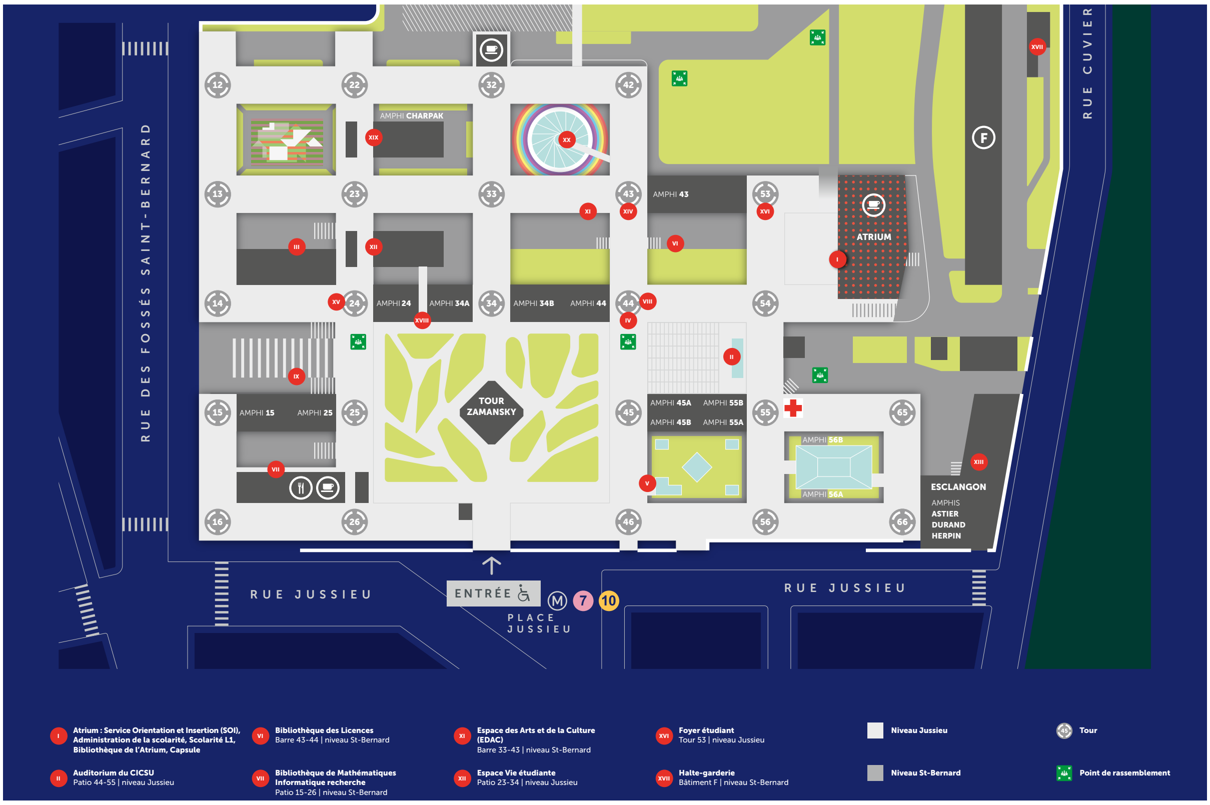
Speaker: Fabien Bruneval
Affiliation: Section de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, France

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 orginates 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-definitiveness of the self-energy [3]. We then show how this property can mathematically enforced with an appriopriate 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) and for the Conference Dinner (at La Coupole), 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 reachable 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.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Barre 43-44 | niveau St-Bernard
VII Bibliothèque de Mathématiques Informatique recherche
Patio 15-26 | niveau St-Bernard
XI Espace des Arts et de la Culture (EDAC)
Barre 33-43 | niveau St-Bernard
XII Espace Vie étudiante
Patio 23-34 | niveau Jussieu
XVI Foyer étudiant
Tour 53 | niveau Jussieu
XVII Halte-garderie
Bâtiment F | niveau St-Bernard
Niveau Jussieu
Niveau St-Bernard
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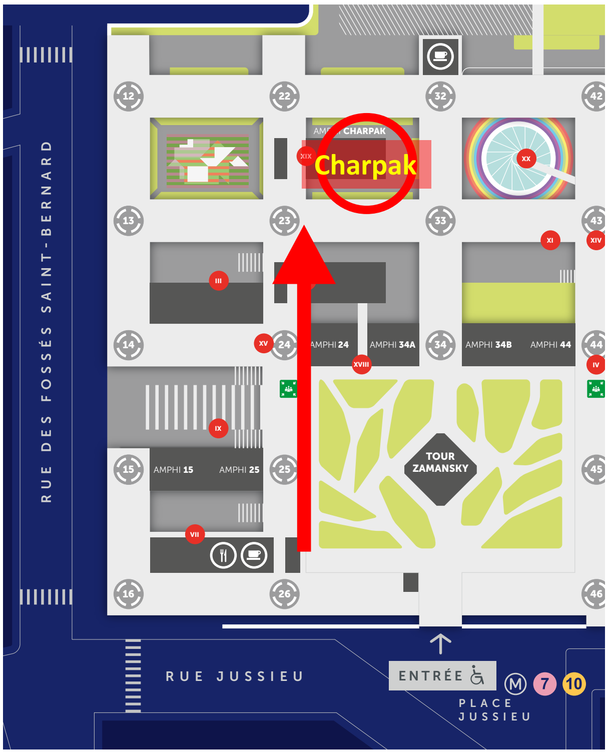
Point de rassemblement

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 main quad: “RdJ”), one goes downstairs (basement level: “RdC”), get out of the Tower and walk towards Tower 22. The entrance of the Charpak lecture hall is on the left: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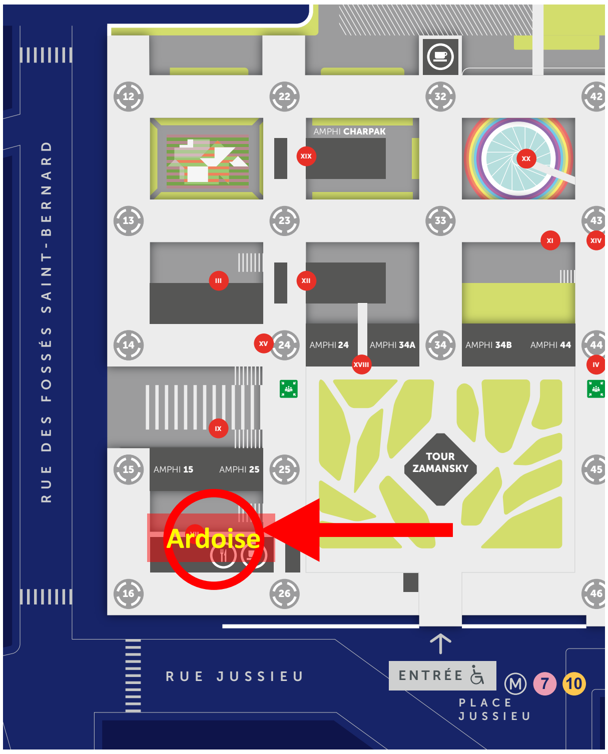
The lunches on November 6 and 7 will be served at the restaurant L’Ardoise, located on campus, at the Jussieu level, as shown below: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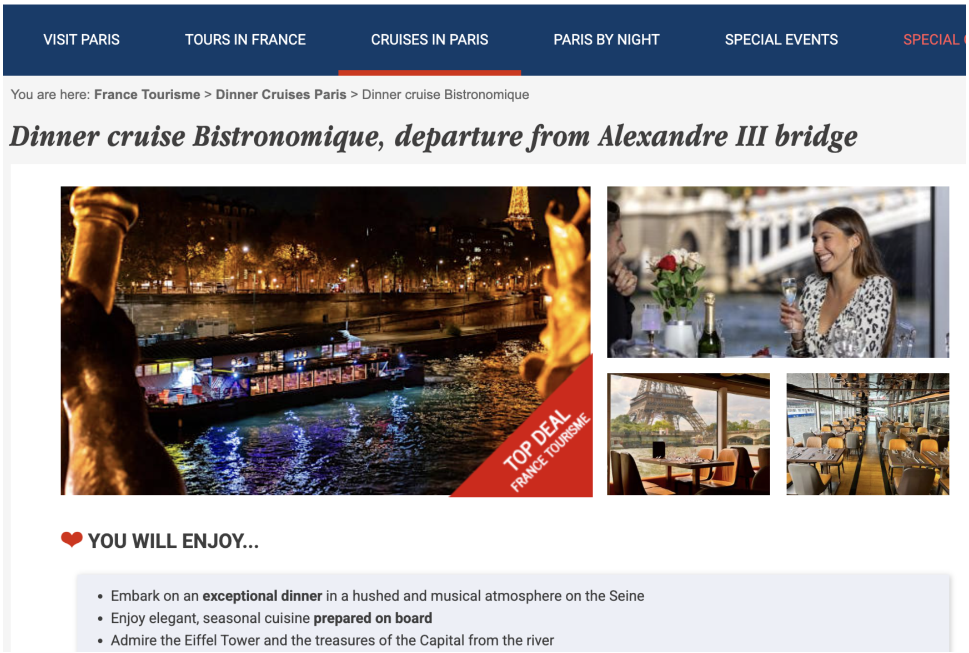
The dinner cruise flyer by France Tourisme: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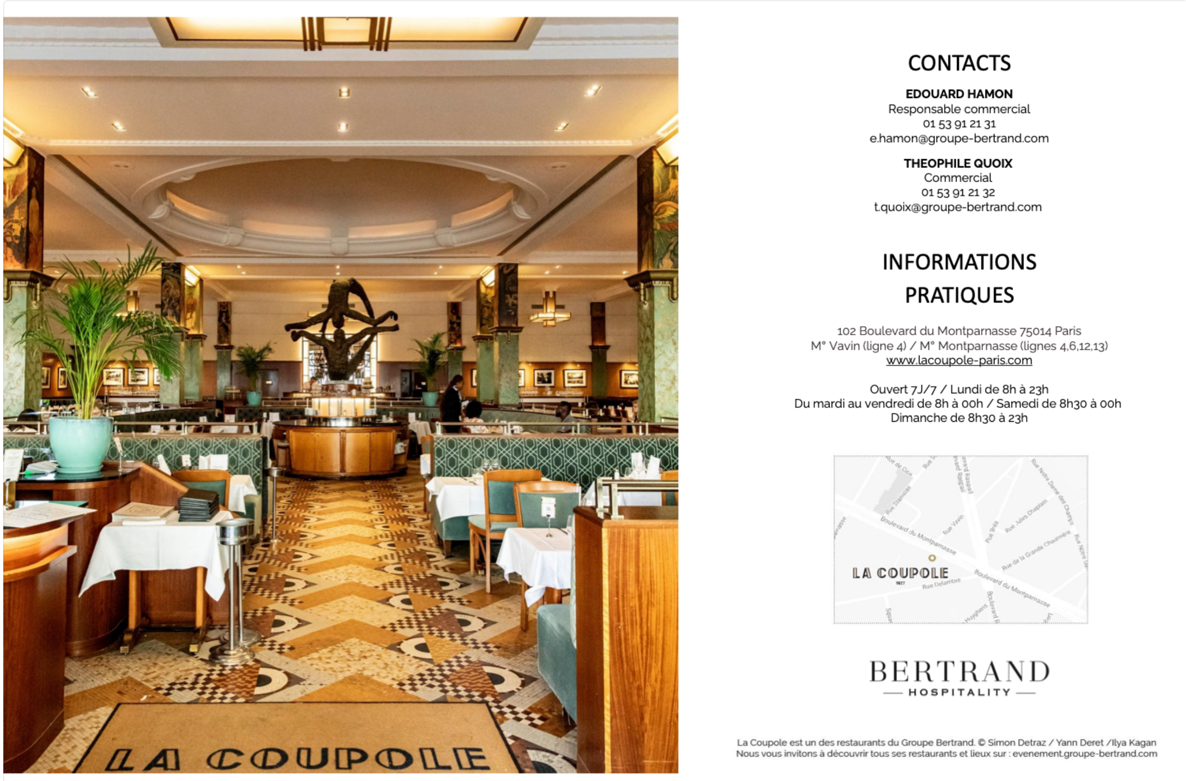
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the European Union

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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, preceding the workshop. 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 during the skill-building days.

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.