

Interdisciplinarity conference on many-body theory

Third general congress of the NBODY research network

Nancy — June 16 to 18, 2025

N-body problem in quantum chemistry, condensed matter physics, nuclear physics, and mathematics



INTERDISCIPLINARITY CONFERENCE ON MANY-BODY THEORY

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I. Presentation of the NBODY research network, and aim of this congress

The NBODY research network was created in January 2019. It aims at bringing together the community working on the N -body problem from the viewpoint of quantum chemistry, condensed-matter physics, nuclear physics, and mathematics. The idea is to foster the development of new computational methods in quantum mechanics, the transfer of these methods from one discipline to another, and their efficient computer implementations. To reach this goal, the research network organizes interdisciplinary conferences and workshops. It is also particularly involved in training students and researchers *via* the organization of several interdisciplinary international schools. The NBODY research network has a web site that can be accessed by clicking [\[here\]](#).

As for the first two general NBODY congresses, the aim of this event is to reinforce the already existing collaborations, and to support the initiation of new ones. Another goal is to favor the integration of PhD students, postdocs, and young researchers in the community. Finally, we would like to facilitate the dialogue between the different topics by including presentations with a pedagogical perspective.

II. General information and venue

Campus: *Faculté des Sciences et Technologies, Vandoeuvre-lès-Nancy*

Building: *Victor Grignard*

Lecture room: *Amphi VG8*

II.1 Reaching Nancy

The town of Nancy can be reached through two railway stations of the French national railway company — the SNCF (check their [\[web site\]](#) for ticket reservation) — : the “Nancy gare SNCF” located at the city-center; or the “Lorraine TGV” station with a connection bus line toward the city center of Nancy. The “Nancy Gare SNCF” in the city center is actually located at 1h30 by train from Paris and Luxembourg.

The three closest airports are the [\[Luxembourg airport\]](#), the [\[Bâle-Mulhouse airport\]](#), and the [\[Lorraine airport\]](#). The Lorraine airport is located between Nancy and Metz.

II.2 Reaching the campus

The lectures will take place on the “campus de la faculté des sciences et technologies de Nancy”. The campus can be reached from the city center using one of the two following local public transport lines:

(i) the Tempo 3 (**T3**) line from the city center (for example, from the “Tour Thiers Gare stop”) in the direction of Villers Campus Science. The building is next to the terminus stop;

(ii) the Tempo 1 (**T1**) from the city center (for example, from the “Gare — Pierre Semard” stop) in the direction of Vandoeuvre Brabois-Hôpitaux. The campus is next to the “Vélodrome-Callot” and the “Le Reclus” stops.

You can consult the map of the public transport network of Nancy (STAN) by clicking [[here](#)]. The schedules files for the T3 and T1 lines can be consulted by clicking [[here](#)]. For each of these lines, the period of interest for us is the Green one (*Période verte — semaine scolaire, du lundi au vendredi*). For your information, the two target schedule files [extracted on April 28, 2025] are also given at the end of this document.

II.3 Reaching the lecture room

The lectures will take place in the Victor Grignard building, in the VG8 amphitheater (“Amphi VG8”). A map of the campus and a map of the building are given at the end of the present document.

II.4 Before and during the lectures

We leave it to the participants to arrange their own accommodation. In case of emergency, please reach this phone number: 0033 625 899 778. Do not hesitate to use the local-contact e-mails of [[Séverine Bonenberger](#)], [[Thibaud Etienne](#)] or [[Jérémy Morere](#)] in case you have any question.

III. Registration and abstract submission

III.1 Registration

For organizational purposes, registration to the school is free of charge but mandatory. Please send an e-mail to [NBODY2025@proton.me]. In your registration e-mail, please provide us with the following:

1. FIRST NAME
2. LAST NAME
3. AFFILIATION

Registration is open until **June 2, 2025** in the limit of a hundred participants.

III.2 Abstract submission

Abstract submission for a contributed talk is now closed. Abstract submission for a poster presentation is still open until **June 2, 2025**. You can download the template you need for your request (poster presentation), either in the Word or LaTeX format, at the following link: [[LINK](#)]. To submit your abstract, please send it to the following e-mail address: [NBODY2025@proton.me].

IV. Schedule and abstracts

In the following table, “IT–XX” means “Invited talk XX” and “CT–XX” means “Contributed talk XX” with the number (XX) corresponding to the number of the abstract in this booklet.

<i>Day 1</i>	<i>June 16, 2025</i>		<i>Amphi VG8</i>
12h00	<i>Organizing committee</i>		Welcoming cocktail
13h30	Matteo Gatti		IT-01
14h00	Marios-Petros Kitsaras		CT-01
14h30	Christian Schilling		IT-02
15h00	Michael Herbst		IT-03
15h30		Coffee break	
16h00	Ewa Pastorczak		IT-04
16h30	Stéphanie Egome Nana		CT-02
17h00	Fabris Kossoski		IT-05
17h30	Jérémie Morere		CT-03
18h00		Poster session	
19h00		Dinner	
<i>Day 2</i> <i>June 17, 2025</i>			<i>Amphi VG8</i>
8h30	Lea M. Ibele		IT-06
9h00	Spondon Sarma		CT-04
9h30	Victor Despré		CT-05
10h00		Coffee break	
10h30	Louis Garrigue		IT-07
11h00	Clémentine Barat		CT-06
11h30	Geneviève Dusson		IT-08
12h00	Clément Guillot		CT-07
12h30		Lunch	
14h00	Mikael Frosini		IT-09
14h30	Guillaume Hupin		IT-10
15h00	Michael Urban		IT-11
15h30	Elias Khan		IT-12
16h00		Coffee break	
16h30	Benjamin Lenz		IT-13
17h00	Stefano Paggi		CT-08
17h30	Carlos Mejutos-Zaera		IT-14
18h00	Carlos Rodriguez-Perez		CT-09
18h30		“Apéro” and Dinner	
<i>Day 3</i> <i>June 18, 2025</i>			<i>Amphi VG8</i>
8h30	David Ferenc		CT-10
9h00	Timothée Audinet		CT-11
9h30	Ryan Benazzouk		CT-12
10h00	André Gomes		CT-13
10h30		Coffee break	
11h00	Pauline Colinet		IT-15
11h30	Emmanuel Giner		CT-14
12h00	Hélène Bolvin		IT-16
12h30	Saad Yalouz		IT-17
13h00		Lunch and departures	

Connector theory: an ecological approach for the design of systematic approximations

IT-01

by Ayoub Aouina^{1,3}, Muhammed Güneş^{2,3}, Matteo Gatti^{2,3*,†}, and Lucia Reining^{2,3}

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One of the main reasons of the computational efficiency of density functional theory is the availability of simple functionals [1], such as the LDA and the GGAs, that make use of interpolated results of highly accurate Quantum Monte Carlo calculations in the homogeneous electron gas [2]. In this way, the LDA and GGAs avoid the drawback that all the results are recalculated entirely from scratch for every material, which is instead the case for orbital functionals or usual approximations of Green's function theory. The recently developed connector theory (COT) [3] generalises, in principle in an exact manner, this successful strategy of importing knowledge from models for the calculation of observables or auxiliary quantities in materials. In practice, COT allows the design of approximations that benefit from error cancelling, are systematically improvable, and constrain the results to be exact in certain limits. In this talk, we illustrate the use of COT for the calculation of the Kohn-Sham exchange-correlation potential [4,5] and the electronic density [6] in prototypical materials.

References

- [1] J. Toulouse, arXiv:2103.02645.
- [2] D. M. Ceperley and B. J. Alder, Phys. Rev. Lett. 45, 566 (1980).
- [3] M. Vanzini, A. Aouina, M. Panholzer, M. Gatti, and L. Reining, npj Computational Materials 8, 98 (2022).
- [4] A. Aouina, M. Gatti, S. Chen, S. Zhang, and L. Reining, Phys. Rev. B 107, 195123 (2023).
- [5] A. Aouina, M. Gatti, and L. Reining, submitted (2025).
- [6] M. Güneş, A. Aouina, V. Gorelov, M. Gatti, and L. Reining, in preparation (2025).

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CONTRIBUTED TALK

Analytic G_0W_0 gradients: An IP/EA-EOM- λ -rCCD reformulation

CT-01

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The G_0W_0 approach is a Green's function method, first developed within the condensed-matter community. Its applications and use in quantum chemistry, however, have grown in recent years. G_0W_0 is used to calculate ionization potentials (IPs) and electron affinities (EAs) beyond Koopman's theorem. It achieves this by including correlation through a dynamically-screened Coulomb interaction derived at the random-phase approximation (RPA) level. Despite formally having an N^6 scaling, this is typically reduced to N^5 using numerical integration. Recent studies show a mean absolute error of 0.31 eV relative to CCSD(T) with a significantly reduced computational cost.[1]

Despite various attempts in the past to derive analytic derivatives for G_0W_0 energies, this has only recently been achieved.[2] The approach takes advantage of the equivalence between the RPA and the ring Coupled-Cluster Doubles (rCCD) approximation.[3] It thus expresses G_0W_0 energies as IP/EA equation-of-motion (EOM) CC solutions on top of a unitary rCCD reference.[4,5] Due to the unitary CC transformation, this approach includes a non-truncating commutator series which is truncated numerically.

In this talk, we present an alternative to the non-truncating unitary rCCD approach. We use a similarity transformation to block-diagonalize the RPA Hamiltonian and use the respective IP/EA-EOM treatment to derive G_0W_0 energies. Lastly, we use the Lagrangian approach to derive an analytic derivative expression, that bypasses the calculation of the parameter response for each different perturbation. We then implemented these developments in a geometry-optimization algorithm to calculation adiabatic IPs and EAs on selected systems.

References

- [1] Marie, A., Ammar, A. & Loos, P.-F. The GW approximation: A quantum chemistry perspective. *in Advances in Quantum Chemistry* vol. 90 157–184 (2024).
- [2] Tölle, J. Fully Analytic G_0W_0 Nuclear Gradients. *The Journal of Physical Chemistry Letters* 16, 3672–3678 (2025).
- [3] Scuseria, G. E., Henderson, T. M. & Sorensen, D. C. The ground state correlation energy of the random phase approximation from a ring coupled cluster doubles approach. *The Journal of Chemical Physics* 129, (2008).
- [4] Quintero-Monsebaiz, R., Monino, E., Marie, A. & Loos, P.-F. Connections between many-body perturbation and coupled-cluster theories. *The Journal of Chemical Physics* 157, (2022).
- [5] Tölle, J. & Kin-Lic Chan, G. Exact relationships between the GW approximation and equation-of-motion coupled-cluster theories through the quasi-boson formalism. *The Journal of Chemical Physics* 158, (2023).

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Entanglement in Identical Particle Systems: Foundation and Applications

IT-02

by Christian Schilling^{1,2}

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Entanglement is a fundamental feature of the quantum world and a key resource for quantum information processing. While the concept of entanglement for distinguishable particles is well established, its validity for identical particles remains a subject of debate and misconceptions. In this talk, we resolve this foundational issue: We demonstrate that identical particles do not form proper subsystems, rendering the concept of entanglement inapplicable to identical particles in first quantization. However, in second quantization, where the focus shifts from particles to the inherently distinguishable orbitals, entanglement becomes well-defined. We then systematically apply this perspective to physics and chemistry. In particular, we show how this framework provides a deeper understanding of chemical bonding and we propose a systematic approach to enhancing wave function methods for strongly correlated electron systems. Altogether, these insights highlight the deep connection between quantum information and quantum many-body physics, demonstrating fruitful synergies that can foster the second quantum revolution.

References

- [1] D. Aliverti-Piuri, J. Liebert, C. Schilling, *forthcoming*.
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INVITED TALK

Efficient and flexible computation of response properties in density-functional theory

IT-03

by Michael F. Herbst^{1*,†}, Niklas Schmitz¹, Bonan Sun^{1,2}

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Computation of response properties, such as dipole moments, spectra or vibrational couplings) are ubiquitous in computational science and important avenues to connect theoretical simulations to experimentally observable quantities. However, more recent efforts in inverse materials design or the quantification of uncertainties in simulations require more unusual DFT derivatives, including responses with respect to a change of structure or DFT functional. Here, algorithmic differentiation (AD) techniques offer great promise to simplify the practical computation of such derivatives. In principle, using AD techniques any derivative of an output quantity (band structure, force, dipoles) with respect to any input quantity (structure, DFT functional, pseudopotential) can be computed.

Over the past years we spend considerable effort equipping the density-functional toolkit (DFTK, <https://dftk.org>) with such algorithmic differentiation capabilities. I will present on recent progress in terms of efficient and reliable algorithms to compute DFT responses and provide some examples illustrating the current state of AD in DFTK.

References

- [1] M. F. Herbst and N. Schmitz, *What gradients can do for you in plane-wave DFT* (in preparation).
- [2] M. F. Herbst and B. Sun, *Efficient Krylov methods for linear response in plane-wave electronic structure calculations*. [arXiv 2505.02319](https://arxiv.org/abs/2505.02319).
- [3] E. Cancès, M. F. Herbst, G. Kemlin, A. Levitt and B. Stamm, *Lett. Math. Phys.* **113**, 21 (2023). DOI [10.1007/s11005-023-01645-3](https://doi.org/10.1007/s11005-023-01645-3).

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INVITED TALK

Molecular properties from adiabatic connection approaches based on the extended random phase approximation

IT-04

by Ewa Pastorcza^{1*,†}, Katarzyna Pernal¹, Michał Hapka,² Szymon Danielski¹ and Daria Drwal¹

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Combining the descriptions of static and dynamic correlation in a balanced and cost-effective way is one of the key challenges of modern-day quantum chemistry.

Static correlation is often captured by employing a multireference wavefunction, e.g., from the Complete Active Space (CAS) Self-Consistent Field approach. The dynamic correlation can be obtained using perturbation methods (most commonly CASPT2 and NEVPT2), but also by the recently proposed adiabatic connection (AC) fluctuation-dissipation approaches combined with the Extended Random Phase Approximation (ERPA).[1,2]

We have shown that the AC-ERPA methods for the excitation energies perform comparably to the popular NEVPT2 method while their computational cost scales more favorably with the number of active orbitals.[3,4]

Here, we show that the AC-ERPA methods are capable not only of correctly describing the ground and excited-state energies of molecular systems, but also of describing their properties, such as the oscillator strengths for electronic transitions and polarizabilities.

While the former are captured by AC-ERPA and its more cost-efficient variant, AC0-ERPA, with impressive accuracy [5], the latter are significantly underestimated. We show how one can alleviate that problem through the employment of a range-separated approach involving both AC-ERPA and density functional theory.

References

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- [2] E. Pastorcza, K. Pernal, *J. Chem. Theory Comp.* 14, 7, 3493–3503 (2018).
- [3] E. Pastorcza, M. Hapka, L. Veis, K. Pernal, *J. Phys. Chem. Lett.* 10, 16, 4668–4674 (2019).
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CONTRIBUTED TALK

Use of Complex Gaussian-Type Orbital expansions for two-center continuum states: Application to H₂⁺ photoionization differential cross sections

CT-02

by S. Egome Nana[†], A. Leclerc , and L. U. Ancarani

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We aim at describing the continuum states of a molecule using complex Gaussian-type orbitals (cGTOs), that is to say GTO with complex exponents. The description of these states is crucial, for example, in the study of molecular ionization processes. However, several challenges arise due to the inherently oscillatory infinite range and multicentric nature of their wavefunctions.

In molecular systems, the evaluation of electronic matrix elements is complicated by the presence of multiple atomic centers. For bound states, this issue can be mitigated using quantum chemistry methods based on GTOs, whose mathematical properties facilitate the computation of multicenter integrals. While many methods and tools have been developed to describe bound states of molecules, equivalent and efficient approaches are not readily available for continuum states.

For continuum states in one-center ionization problems, only one oscillatory radial function is required. Ammar *et al.* [1,2] proposed to use cGTOs sets for its numerical representation. This approach has been proven effective on extended radial domains [3], and allows for analytical integral calculations applicable to ionization processes [1,2].

In a multicentric framework, continuum states are not well mastered; the evaluation of matrix elements in this context presents considerable difficulties. As a contribution to the field, we wish to extend the cGTO approach to handle multiple centers, starting with the treatment of the two-centers case. For the final state, we consider the Two-Center Continuum (TCC) model [4] proposed to describe the continuum states of an electron ejected with momentum \mathbf{k}_e during the ionization of one-electron diatomic targets. The model wavefunction is given by:

$$\chi(\mathbf{r}_1, \mathbf{r}_2) = \frac{e^{i\mathbf{k}_e \cdot \mathbf{r}}}{(2\pi)^{3/2}} C(\mathbf{k}_e, \mathbf{r}_1) C(\mathbf{k}_e, \mathbf{r}_2) \quad (1)$$

where \mathbf{r}_1 and \mathbf{r}_2 are the position vectors with respect to the two centers, $\mathbf{r} = (\mathbf{r}_1 + \mathbf{r}_2)/2$, and $C(\mathbf{k}_e, \mathbf{r}_1)$ and $C(\mathbf{k}_e, \mathbf{r}_2)$ represent analytically known distortion functions. The wavefunction $\chi(\mathbf{r}_1, \mathbf{r}_2)$ captures the essential features of the bicentric continuum.

As a first application we have considered the photoionization of H₂⁺. Its ground state is expanded on standard GTO while the TCC is represented with cGTO expansions. Cartesian coordinates are used since they facilitate the evaluation of integrals. With these two expansions, we have obtained a closed-form expression of the scattering amplitude. The numerical implementation of our Gaussian approach is benchmarked with previously published cross sections.

References

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Resonances and the complex absorbing potential method

IT-05

by Fábris Kossoski¹

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Unlike electronic bound states, resonances are metastable states that decay by loss of an electron. Their unbound character introduces an additional layer of complexity to the quantum many-body problem. In this presentation, I will review the main approaches to model resonances, which can be grouped into scattering methodologies and adapted quantum chemistry methods. Belonging to the latter class, I will discuss in more detail the complex absorbing potential (CAP) method, which regularizes the resonance wave function by introducing an imaginary potential that acts in the asymptotic region. This is one of the most popular approaches thanks to its comparatively easier computational implementation. The CAP method has been combined with various levels of electronic structure theory, ranging from equation-of-motion coupled-cluster to multiconfigurational methods, and, more recently, with selected configuration interaction. Although the latter implementation now allows the full configuration interaction limit of resonances to be reached, the errors associated with the finite basis set and with the CAP itself remain less understood. I will present recent results that addresses the interplay of these two sources of error, and the unexpected consequences associated with the optimization of the CAP strength.

References

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CONTRIBUTED TALK

Catalan numbers, Dyck language, and second quantization: An algorithm-oriented representation of second quantization chains CT-03

by Jérémie Morere^{1*,†}, and Thibaud Etienne¹

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Second quantization is a fundamental formalism in quantum chemistry and condensed matter physics for describing systems of bosonic and fermionic particles. For electrons, this formalism enables the systematic manipulation of Slater determinants and operators representing observables, based on the anti-commutation and hermiticity rules of creation and annihilation operators. Second quantization operators are used in methods to describe many-body systems, such as coupled-cluster theory or configuration interaction.

Evaluating the expectation value of a chain of second quantization operators is a central challenge. Wick's theorem makes it possible to simplify the evaluation of an expectation value of a chain, relative to a vacuum, by expressing it as the normal order of the chain plus a sum of all contractions of the chain taken in normal order. That expectation value, with respect to the physical or Fermi vacuum, is given by the sum of the expectation values of the fully contracted terms. In fact, the expectation value of any non-fully contracted term is zero. The main advantage of this formulation is that it reduces the problem to finding all fully contracted terms. These terms can be expressed in terms of products of Kronecker deltas. In other words, finding the expectation value becomes a problem of finding viable pairings of second quantization operators. If this procedure is well defined, the number of terms generated by the contractions grows rapidly, making the computations costly in terms of time and memory. In addition, a significant number of the fully contracted terms will be zero, so it seems necessary to find criteria to limit the calculations to the non-zero terms as much as possible.

In this talk we propose a translation of chains of second quantization operators into a Dyck language. A word in a Dyck language can be seen as a string of left and right parenthesis (and/or brackets). If a word corresponds to a balanced string, it is called a Dyck word. In a chain of second quantization operators, each operator is translated into left or right parenthesis. If the resulting string is a Dyck word, the expectation value of the chain is non-zero. Two examples are given below. Let $| \rangle$ denote the physical vacuum:

$$\langle | \hat{a}_{i_1} \hat{a}_{i_2} \hat{a}_{i_3} \hat{a}_{i_4}^\dagger \hat{a}_{i_5}^\dagger \hat{a}_{i_6} \hat{a}_{i_7}^\dagger \hat{a}_{i_8}^\dagger | \rangle \leftrightarrow (())() \quad (1)$$

$$\langle | \hat{a}_{i_1} \hat{a}_{i_2}^\dagger \hat{a}_{i_3} \hat{a}_{i_4}^\dagger \hat{a}_{i_5}^\dagger \hat{a}_{i_6} \hat{a}_{i_7} \hat{a}_{i_8}^\dagger | \rangle \leftrightarrow ()()() \quad (2)$$

At first sight, i.e., before translation, it is not obvious that

$$\langle | \hat{a}_{i_1} \hat{a}_{i_2} \hat{a}_{i_3} \hat{a}_{i_4}^\dagger \hat{a}_{i_5}^\dagger \hat{a}_{i_6} \hat{a}_{i_7}^\dagger \hat{a}_{i_8}^\dagger | \rangle$$

is a non-zero while

$$\langle | \hat{a}_{i_1} \hat{a}_{i_2}^\dagger \hat{a}_{i_3} \hat{a}_{i_4}^\dagger \hat{a}_{i_5}^\dagger \hat{a}_{i_6} \hat{a}_{i_7} \hat{a}_{i_8}^\dagger | \rangle$$

is zero. However, after translation, it is clear that the first string is balanced and the second is not, implying the nullity of the second expectation value. The enumeration of chains of operators with a non-zero expectation value then joins the large family of problems for which Catalan numbers are the solution. This family includes Dyck language, triangulation of polygons, or some graph problems. This analogy makes it possible to formulate non-nullity rules

for the expectation value of chains of operators. At the same time, tools used to describe Dyck words, can be used to predict the number of non-zero terms in the sum after applying Wick's theorem. A similar relationship can be made with respect to the Fermi vacuum, allowing us to work with Slater determinants.

The graphical representation of admissible chains has enabled us to develop an algorithm for symbolically evaluating the expectation value of a 1-body operator between two Slater determinants. The strength of this algorithm is to reduce as much as possible the number of second quantization operator pairings to be taken into account to obtain the result, thus reducing the complexity of the algorithm.

References

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Ab Initio Multiple Spawning Dynamics With Different Flavours of CASPT2

IT-06

by Lea M. Ibele¹

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Nonadiabatic dynamics has become an indispensable tool for unraveling the photochemistry and photophysics of molecules. However, despite the field's growth, it often remains limited to expert users, partly due to the lack of accessible and user-friendly software.

In this talk, I will present our work [1] on propagating nonadiabatic dynamics using the Ab Initio Multiple Spawning (AIMS) method on potential energy surfaces computed at the CASPT2 level enabled by our recently developed interface between PySpawn [2] and OpenMolcas [3]. This combination of user-friendly and fully open-source software allows for the first time running AIMS with different multistate CASPT2 formulations, combining state-of-the-art dynamics and electronic structure calculations. AIMS is widely recognized for its accuracy in simulating nuclear motion on coupled electronic states [4], using trajectory-guided Gaussian wave packets to naturally incorporate nonadiabatic transitions and nuclear quantum effects.

High-quality dynamics require high-quality electronic structure data. OpenMolcas provides access to CASPT2 energies and gradients, often considered the gold standard for multireference systems. Recent advances have introduced improved multistate CASPT2 variants – MS, XMS, XDW, and RMS [5-8] – each with trade-offs between accuracy and smoothness of the potential energy surfaces. MS-CASPT2 excels in vertical excitation energies but may produce discontinuous surfaces near state crossings. XMS offers smooth surfaces at the cost of excitation energy accuracy, while XDW and RMS aim to balance both.

We applied this AIMS/CASPT2 framework to study the excited-state dynamics of fulvene, systematically comparing the CASPT2 variants. Our results reveal significant differences in relaxation pathways depending on the chosen formulation and highlight the impact of second-order corrections. These findings offer practical guidance on selecting the appropriate CASPT2 flavor for accurate and robust nonadiabatic simulations.

References

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Wavefunction propagation at conical intersections: spin separation via spin-orbit coupling

CT-04

by Spondon Sarma^{*,†}, Francesco Talotta, and Lorenzo Ugo Ancarani

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Excited-state, non-adiabatic dynamics are at the core of many challenges in molecular physics, from biological photoreactions to next-generation electronic components and light-responsive materials. Deciphering their mechanisms remains challenging because these processes tightly interweave nuclear and electron motion with subtle quantum effects.

A central manifestation of this complexity is represented by the set of radiation-less pathways that let an excited molecule shed energy without emitting light, such as internal conversion (IC), which takes place between electronic states of the same spin multiplicity, driven by nonadiabatic nuclear-electronic couplings. By contrast, Intersystem crossing (ISC) moves population between states of different spin multiplicities through relativistic spin-orbit coupling (SOC). Unraveling the balance and interplay between IC and ISC is pivotal for predicting photo-stability, tuning photosensitisers, and engineering molecular devices that exploit excited-state dynamics. Moreover, a recent study [1] has demonstrated that spin effects can be crucial in steering nuclear dynamics near conical intersections (CI). This effect could have significant implications for the dynamics of radical molecules, the design of spintronics devices, and for understanding spin-dependent chemistry.

In this contribution, we will show how the novel generalized coupled trajectory mixed quantum/classical (G-CT-MQC) [2] method, based on the exact factorization theory, can be used to study the nuclear molecular dynamics where both non-adiabatic and spin-orbit coupling are present. Our simulations show how a nuclear configuration initially prepared on a single electronic state for a two-state 2D model (with IC and ISC) evolves as it approaches a CI, and how the SOC near the CI induces preferential selection of specific outgoing channels based on the electronic spin. A critical assessment of the quantum/classical G-CT-MQC method is made by qualitatively and quantitatively comparing transmission rates and spin selectivity with results obtained within a time-dependent full quantum mechanical approach.

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CONTRIBUTED TALK

Correlation-Driven Charge Migration Triggered by Infrared Multi-Photon Ionization

CT-05

by Victor Despré

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In a molecular system, the correlation-driven charge migration [1] (CDCM) is a purely electronic process that involves the ultrafast dynamics of electrons originating from coherent superposition of eigenstates followed by the ionization of a single molecular orbital [2]. The possibility of observing CDCM has been a driving force behind theoretical and experimental developments in the field of attosecond molecular science since its inception. Although X-ray free-electron lasers have recently emerged as a promising tool for experimentally observing CDCM, the unambiguous observation of CDCM, or more generally, charge migration dynamics triggered by ionization, remains elusive.

In this work [3], we present a method to selectively trigger such dynamics using molecules predicted to exhibit long-lived electron coherence. We show that these dynamics can be selectively triggered using infrared multi-photon ionization and probed using the spacial resolution of X-ray free-electron laser, proposing a promising experimental scheme to study these pivotal dynamics. Additionally, we demonstrate that real-time time-dependent density-functional theory can describe correlation-driven charge migration resulting from a hole mixing structure involving the HOMO of a molecule.

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INVITED TALK

Coupling the variational approximation and perturbation theory

IT-07

by Louis Garrigue¹

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To approximate eigenvalue problems, one can reduce the exact total variational space to a subspace, this is often called the variational approximation. A special choice of subspace is the one spanned by the vectors extracted from perturbation theory, i.e. the coefficients of the eigenvector Rayleigh-Schrödinger Taylor series. We give an analysis, rigorous bounds, and compare quantitatively the performance of the approach with perturbation theory alone. This method provides a general, natural and efficient way of approximating eigenmodes.

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CONTRIBUTED TALK

Preconditioning the self-consistent field for magnetic systems in Kohn-Sham density functional theory

CT-06

by Clémentine Barat^{1, 2, 3, †}, Antoine Levitt³, and Marc Torrent^{1, 2}

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Kohn-Sham density functional theory is a widely used method in solid state physics and chemistry for simulating the electronic properties of materials. The Kohn-Sham equations can be reduced to a fixed-point problem and are generally solved using self-consistent iterations. For complex systems, convergence is highly dependent on the mixing scheme and preconditioner used. A notable challenge arises in magnetic systems, where the Jacobian of the fixed-point equation can have an eigenvalue close to zero, leading to convergence problems.

Here, we present a parameter-free preconditioner for the self-consistent field designed to overcome convergence issues in magnetic systems.

[†] Speaker

INVITED TALK

Guaranteed Error Bounds in Electronic Structure Calculations

IT-08

Geneviève Dusson^{*,1}

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Université de Franche-Comté*

Simulating the electronic structure of molecular systems requires solving nonlinear eigenvalue partial differential equations (PDEs). In practice, these equations are solved approximately, by discretizing the PDEs and then solving the resulting discrete equations using an iterative algorithm.

In this talk, I will present guaranteed and computable error bounds for the solutions of such PDEs. The goal of this work is to estimate the error between the exact solution of the PDE and the numerically computed approximate solutions, in order to ensure the accuracy of the obtained results. I will highlight two main contributions in particular: guaranteed error bounds for the (nonlinear) Kohn-Sham equations in density functional theory, and guaranteed error bounds for linear eigenvalue problems discretized using localized basis functions.

CONTRIBUTED TALK

Low-complexity approximations with least-squares formulation of the time-dependent Schrödinger equation

CT-07

by Mi-Song Dupuy¹, Virginie Ehrlacher², and Clément Guillot^{2,†}

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²*École Nationale des Ponts et Chaussées, Inria*

Solving the Schrödinger evolution equation numerically poses significant challenges due to the inherent high dimensionality of the solution space. This presentation introduces a novel reformulation of the evolution problem as the minimization of a quadratic space-time functional. This approach enables the computation of solutions using nonlinear ansatz functions. We demonstrate the effectiveness of our method through numerical experiments employing specific ansatz, such as low-rank formats and free Gaussian wave packets.

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† Speaker

Taming down the complexity of the nuclear many-body problem

IT-09

by Mikael Frosini¹ ^{†,*}, Thomas Duguet^{2,3}, Stavros Bofos¹, and Lars Zurek^{4,5}

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The development of predictive models for atomic nuclei from first principles is a challenging yet essential endeavor to generate systematic theoretical predictions and associated uncertainties. Ab initio methods are particularly promising as they provide controlled and systematically improvable approximations for both inter-nucleon interactions and solutions to the many-body problem. However, solving the many-body Schrödinger equation in heavy open-shell systems typically involves constructing and repeatedly storing large tensors, posing significant technical challenges.

In closed-shell nuclei, symmetry-restricted calculations can mitigate the computational cost of handling these tensors. Unfortunately, this approach is not feasible for open-shell systems—which constitute the vast majority of nuclei—where allowing symmetries to break spontaneously at the mean-field level is crucial to capture strong correlations at a polynomial cost with system's size. This, in turn, necessitates managing large, dense tensors.

In this presentation, I will illustrate the computational bottlenecks inherent to the theoretical description of open-shell systems. Furthermore, I will introduce dimensionality reduction strategies designed to alleviate memory and runtime constraints, thereby enhancing the efficiency of these calculations.

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INVITED TALK

A primer on *ab initio* complex scaling method for light nuclear systems

IT-10

by Guillaume Hupin^{1,*†}, Osama Yaghi¹

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We present a novel *ab initio* many-body method designed to compute the properties of nuclei in the continuum. This approach integrates well-established techniques, specifically the No-Core Shell Model (NCSM), the Similarity Renormalization Group (SRG), and Complex Scaling (CS) methods. We demonstrate that this combination effectively overcomes the numerical limitations previously encountered.

To benchmark the method, we apply it to the $A = 4$ systems and show that, by employing adequate extrapolation techniques with respect to the new hyperparameter, we can recover exact results consistent with few-body techniques. This work paves the way for applying these methods to heavier mass systems, providing a reliable representation of the initial Hamiltonian and its continuum properties.

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INVITED TALK

Superfluidity: from cold atoms to neutron stars

IT-11

by Michael Urban^{1,*†}

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In this introductory talk, I will give a rapid overview of superfluidity in ultracold trapped Fermi gases and in neutron stars. After highlighting the common features and differences of these two systems, I will present a way for computing the pairing gap in ultracold atoms and the equation of state of dilute neutron matter beyond mean-field theory, based on Bogoliubov Many-Body Perturbation Theory (BMBPT). Finally, I will address the question of superfluid density in the inhomogeneous (crystalline) phase of the inner crust of neutron stars, where the “geometric contribution” that was recently introduced in condensed-matter systems (multiband superconductors) plays a crucial role.

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On the relevance of quantality in atomic nuclei and many-body systems

IT-12

by J.-P. Ebran^{1,2}, L. Heitz³, and E. Khan^{3,4*,†}

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The use of quantality is discussed in the case of nuclei and other many-body systems. This dimensionless quantity is known to indicate when a many-body system behaves like a crystal or a quantum liquid. Its role is further analyzed by showing its relation to the scattering length. The occurrence of a cluster phase in nuclei is analyzed using the quantality through its relation to the localization parameter, allowing for the identification of both the number of nucleons and the density as control parameters for the occurrence of this phase. The relation of the quantality to the magnitude of the interaction also exhibits a third dimensionless parameter, monitoring the magnitude of the spin-orbit effect in finite systems. The impact of quantality on the spin-orbit effect is compared in various many-body systems. Nuclei are found to be exceptional systems because all their dimensionless quantities are close to the order of unity, at variance with other many-body systems.

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INVITED TALK

Studying strongly interacting systems by quantum cluster techniques using a matrix-product state based cluster solver

IT-13

by Benjamin Lenz¹

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In order to describe salient features of strongly correlated materials, e.g. with respect to photoemission spectra, dynamical mean-field theory (DMFT) and its cluster extensions have proven to be well suited techniques. The methods of choice to calculate the central object within them, the (cluster) Green's function, are often quantum Monte Carlo (QMC) solvers, which provide a precise description at finite temperature, but often suffer from the fermionic sign problem. An alternative class of solvers which avoid this problem are based on exact diagonalization (ED). However, the system size that can be treated, be it in terms of cluster or bath sites, is very limited. This limit of applicability can be extended by resorting to efficient compression schemes linked to matrix-product states (MPS).

In my talk, I will first illustrate at the example of tetragonal CuO the complementary aspect of using QMC and MPS-based solvers for cluster-DMFT calculations^[1]. I will then present a MPS-based band Lanczos solver, which allows to calculate the cluster Green's function on cluster geometries well beyond the reach of ED methods^[2]. At the end of my talk I will also show results for its application to the calculation of x-ray absorption spectra for strongly correlated materials, building on an ab initio DFT+DMFT description.

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-

Multi-Channel Dyson Equation: Coupling many-body Green's functions

CT-08

by Stefano Paggi^{1,*†}, J. Arjan Berger², and Pina Romaniello^{1,*}

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We have recently introduced the concept of the multichannel Dyson equation (MCDE) as an alternative to the standard single-channel Dyson equation.[1-3] While the latter involves a single many-body Green's function, the MCDE uses a multichannel Green's function in which two or more many-body Green's functions are coupled. To demonstrate its advantages, the MCDE has been applied to the coupling of the one-body Green's function (1-GF) and the three-body Green's function (3-GF) to calculate direct and inverse

photoemission spectra. This coupling naturally puts quasiparticles and satellites on an equal footing, contrary to the single-channel Dyson equation for the 1-GF, and, therefore, accurate results could be obtained from relatively simple approximations to the multichannel self-energy. For example, a static multichannel self-energy only containing the bare Coulomb interaction yields exact spectral functions of the symmetric Hubbard dimer [2], contrary to standard methods such as *GW* or the T-matrix approximation.

An H_2 -like model at 1/2-filling has also been investigated, yielding also very promising results. In the same spirit, the neutral excitation energies of a helium-like two-level model have been calculated by coupling the two- and four-body Green's functions[4]. The four-body space aids the description of double excitations, which are currently difficult to capture within standard ab-initio methods.

In general the MCDE offers a natural framework to couple excitations and therefore it can describe additional spectral features that are not present at the non-interacting level, such as plasmon and double-plasmon excitations, or biexcitons.

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Quasiparticle Based Embedding for Correlated Electrons: the Ghost Gutzwiller Ansatz

IT-14

by Carlos Mejuto Zaera^{1,†}¹*Laboratoire de Physique Théorique, CNRS, Université de Toulouse, UPS, 118 Route de Narbonne, F-31062 Toulouse, France.*

Strong electronic correlation underlies the stabilization of remarkable phases of matter in materials characterized by their tuneability in terms of external parameters, such as temperature and pressure. Leveraging these features for device design calls for theoretical models which are both accurate and easy to interpret. Embedding frameworks aim to answer this call by mapping the system under study into a smaller impurity problem. Among them, the ghost Gutzwiller (gGut) Ansatz has recently emerged as a promising formalism which seemingly realizes a provocative ideal: obtaining a band structure theory for correlated electrons. At its core, gGut is a variational wave function method generalizing the Gutzwiller Ansatz, which can be equivalently formulated as a self-consistent local embedding within an infinite dimensional approximation. The underlying many-body wave function consists of a Slater determinant and a projector operator, the former obtained as the ground state of a quasiparticle model. Crucially, by adding auxiliary orbitals in this model, the eponymous ghosts, it becomes possible to model strongly correlated phenomena in terms of one-body fluctuations in the enlarged Hilbert space. In this talk, I will review the basic structure of the formalism, and discuss some sample results in model and *ab initio* calculations, showing how gGut can capture photoemission spectra directly from the quasiparticle Hamiltonian, recover non-local interactions rigorously in the embedding, as well as provide simple interpretative pictures for complex manifestations of electron correlation.

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CONTRIBUTED TALK

Accurate observables from Quantum Monte Carlo for solids and molecules

CT-09

by Carlos Rodriguez Perez^{†*}, Francesco Sottile, and Vitaly Gorelov
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The one body reduced density matrix (1RDM) is a many-body object without a classical equivalent. It tells us a lot about the degree of correlation in the system, particularly how electrons occupy the single particle states [1]. We have computed this object with Quantum Monte Carlo techniques for two systems. First, we have benchmarked the accuracy of QMC-1RDMs and densities, comparing them with the exact solution of the Helium atom, answering the questions 'Does a better QMC energy imply better observables?' and 'What is the best and the most efficient way to compute different observables?' with a focus on the density and reduced density matrix. Most recently we have computed accurate RDMs for crystalline Silicon by treating the problem of finite system size. This now allows us to compute reliable RDMs for crystalline systems.

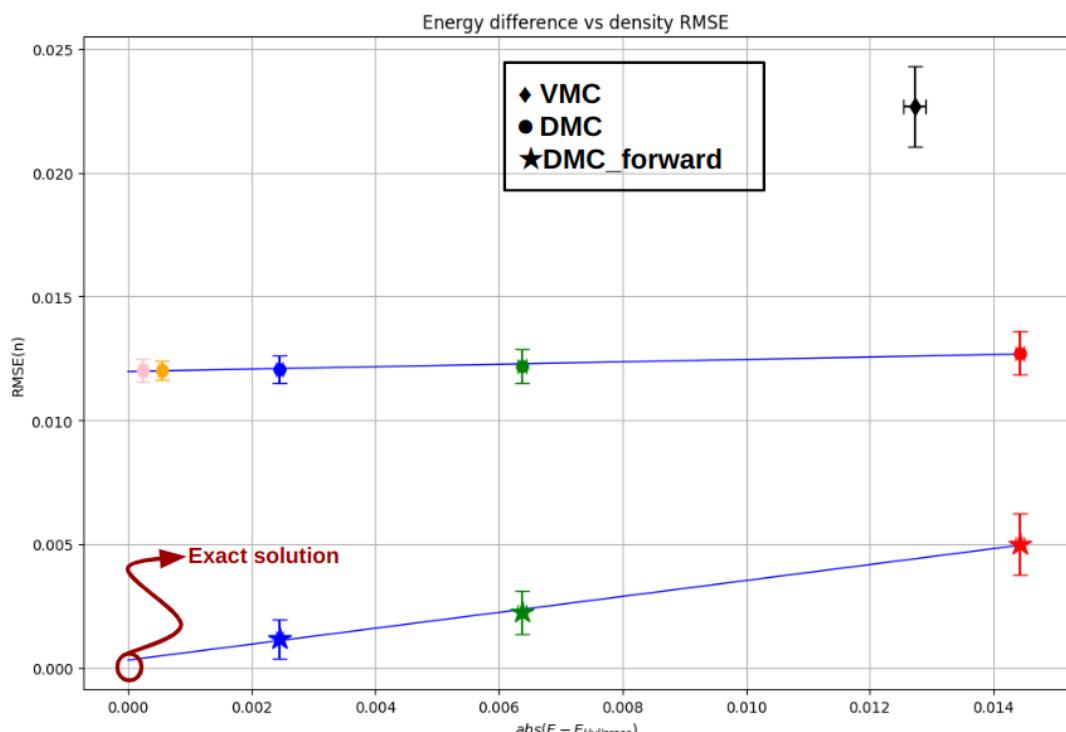


Figure: Root Mean Square Error of the density against the energy difference of the corresponding calculation. The colors indicate the time steps, and as we move left in the figure they are roughly halved with respect to the previous one. Mixed estimator DMC does not yield exact densities in the zero time step limit. Forward walking allows us to compute QMC densities that go to the exact result for zero time step. [2]

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CONTRIBUTED TALK

Gaussian basis set approach to one-loop self-energy

CT-10

by Dávid Ferenc^{1,*†}, and Trond Saue¹

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The accurate computation of QED corrections to the energy levels of molecules, to all-orders in the external Coulomb potential, presents a significant challenge. The use of Gaussian basis sets is an essential ingredient in extending such calculations to polyatomic molecular systems. At the one-loop level, the corrections to the electron-nucleus interaction are vacuum polarization and the electron self-energy. The leading-order (in $Z\alpha$) vacuum polarization correction can be included in molecular computations as an effective local potential (Uehling potential) [1]. The computation of the complete many-potential vacuum polarization density was carried out recently in a Gaussian basis set [2]. The evaluation of the self-energy correction on the other hand is more involved. In this contribution, I present a method that combines the rigorous bound-state QED approach, the many-potential expansion, with a Gaussian basis set expansion to obtain accurate values for the one-loop self-energy correction in a hydrogen-like atom [3].

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[†] Speaker

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Development of a relativistic one-dimensional model including quantum electrodynamics effects

CT-11

by Timothée Audinet^{1,†}, Julien Toulouse^{1,2,*},

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It is important to take into account the effects of special relativity in the quantum description of chemical systems with heavy elements. The relativistic effects account for gold's color, mercury's liquid state at room temperature and are responsible for the efficiency of lead-acid batteries in cars [1]. Relativistic electronic-structure computational methods have been developed in the no-pair approximation, and are now routinely applied on molecular systems. Hence, the next challenge is to go beyond the no-pair approximation by including the quantum-electrodynamics (QED) effects of virtual electron-positron pairs. Such description is needed to recover some properties, even in very simple systems, e.g. the Lamb shift in the Hydrogen atom.

In this work we are interested in a one-dimensional model of relativistic hydrogen-like atom using delta-potential interactions. It is motivated by the non-relativistic version of this model which leads to the same ground-state energy and radial wave function as the three-dimensional one [2]. In this model we are able to make accurate QED calculations [3,4]. After calculating the spectrum of the 1D Dirac operator [5]

$$\mathbf{D}(x) = -ic\sigma_1 \frac{d}{dx} + \sigma_3 mc^2 - Z\delta(x) \quad (1)$$

in first quantization, we develop it in a finite basis set. This effective QED theory includes the effects of the vacuum polarization but does not include the photon degrees of freedom [6,7,8]. Within this framework we are able to calculate within a finite basis set the vacuum-polarization density and the QED Lamb-type shift of the bound-state energy.

The next step is to use the insights obtained from simple model to tackle the issues of the 3D case.

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[†] Speaker

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CONTRIBUTED TALK

Vacuum polarization in a Gaussian basis set

CT-12

by Ryan Benazzouk^{1,*†}, Maen Salman², and Trond Sæu¹

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Recent developments have raised a new spark of interest for Quantum Electrodynamics (QED), from high-precision experiments to search for physics beyond the Standard Model. For instance, it turns out that high-precision QED calculations for molecules could be of key importance in the search for new physics [1].

However, it is yet unclear to what extent QED is needed to describe those molecular properties. Relativistic effects play a prominent role in molecular systems containing heavy elements, and they can be computed to such high precision that correlation effects become the main source of error. But as correlation methods progress, the point approaches at which those effects compare with the magnitude of QED corrections [2]. One can then wonder if those corrections are relevant to understand molecular structure, or properties of the electronic density in the vicinity of heavy nuclei.

Unfortunately, the S-matrix formalism of QED deals rather poorly with electron correlation, as it requires very high orders of perturbation theory. Therefore, one could aspire to a formulation of the theory that fits closer with the variational apparatus of molecular physics. Thankfully, such a program has already been proposed by Chaix & Iracane [3], and extensively studied by mathematicians [4,5]: the Bogoliubov-Dirac-Fock model. The merit of this approach is that it yields a mean-field effective extension to the Dirac Hamiltonian that includes QED effects, reviving Dirac's interpretation of a negative energy sea, in a formalism akin to quantum chemistry. The QED effects, self-energy and vacuum polarization, arise respectively as an exchange and an electric potential generated by charge distribution in the polarized vacuum.

The goal of the **HAMP-vQED** project is therefore to provide a method for calculating QED effects on the electronic structure of molecules in the framework of quantum chemistry. Effective potentials already exist to target valence electrons, but we suspect that they might not be as reliable for core orbitals that undergo very intense electric fields. To do so, we then aim to compute vacuum polarization density and self-energy corrections using Gaussian-type basis sets. In this contribution, I will present my work on vacuum polarization in a finite basis, and more specifically our results on energy shift calculations.

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† Speaker

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Coupled cluster molecular response properties for heavy element systems

CT-13

by Xiang Yuan¹, Loïc Halbert¹, and André Severo Pereira Gomes^{1,*†}

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Accurate electronic structure calculations have become and indispensable tool to understand the molecular properties of heavy (and superheavy) elements. Such approaches help make sense of the underlying complex physical processes probed by experiments, or in case such experiments are unfeasible (due to hazards such as radiotoxicity, short element lifetimes etc).

In this presentation I will outline our contributions to developments of coupled cluster approaches based on two- and four-component Hamiltonians for the determination of linear [1] and quadratic response theories [2, 3]. In particular, I will discuss the similarities and differences between the standard coupled cluster response theory and its equation of motion (EOM) flavor, for properties involving electric, magnetic and mixed electric-magnetic perturbations.

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INVITED TALK

Advancing Electrostatic Embedded Cluster Methods: Efficient QM/MM via FMM and RI-BUPO-J Algorithms

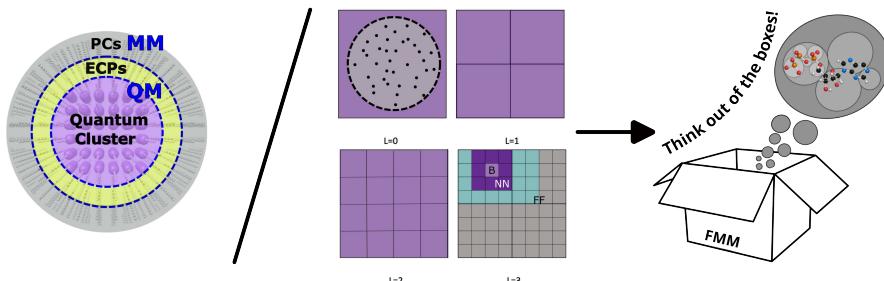
IT-15

by Pauline Colinet^{†,*^{1,2}}, Benjamin Helmich-Paris², Frank Neese²

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Electrostatic embedded cluster (ECM) methods have proven highly effective for modeling semiconductors and insulators, focusing quantum mechanical (QM) calculations on a central cluster while embedding it in a field of point charges (PCs) that approximate the surrounding environment. A surrounding shell of effective core potentials (ECPs) is used to prevent over-polarization of the QM region. This hybrid approach, when combined with accurate quantum chemistry methods, has successfully captured key electronic and magnetic properties of oxide surfaces under catalytic oxidation conditions.

As research progresses toward modeling surface electrocatalysis under operando conditions with atomistic resolution, the need arises for significantly larger QM clusters, typically 200–300 atoms, and electrostatic environments involving up to a million point charges. At this scale, evaluating the electrostatic potential generated by the PCs becomes a major computational bottleneck, with a cost that scales as $O(N_{PC} \times N_{BF}^2)$, where N_{PC} is the number of point charges and N_{BF} the number of basis functions.

To address this, we implemented the long-known Fast Multipole Method (FMM) in the ORCA quantum chemistry package. Indeed, though many quantum chemistry packages are equipped with FMM or have been interfaced with FMM libraries, we believe that adding it to ORCA is a great benefit to the community enabling to couple efficient ECM calculations with ORCA's cutting-edge electronic-structure methods. FMM is a well-established algorithm for accelerating long-range evaluation of electrostatic interaction, which enables to reduce the computational scaling to $O(N_{BF}^{1.25})$, thus significantly speeding up QM/MM calculations. Our initial implementation, focusing on the easiest part, PC/PC interactions, allowed us to fine-tune the algorithm and resulted in over a 10-fold speedup while maintaining micro-Hartree accuracy.

Extending FMM to QM/PC interactions required an efficient multipole treatment of the electronic charge density. By revisiting how atomic orbital shell pairs are processed, we achieved a robust and accurate near-/far-field decomposition, yielding a 10-100× speedup with respect

to ORCA’s previous version (5.0) with accuracy well within chemical thresholds (better than 1 kcal/mol).

Finally, even though not specific to ECM calculations, remain the more complex QM/QM Coulomb interactions, which are known to be difficult to linearize. We developed a new algorithm called RI-BUPO-J (“Bubblepole”). This method combines the resolution-of-identity (RI) approximation with a novel alternative to FMM’s hierarchical boxing: adaptive spherical groupings of basis and auxiliary functions (“bubbles”). RI-BUPO-J provides a flexible and intuitive framework for evaluating Coulomb matrices in large systems. It achieves micro- to nano-Hartree accuracy compared to the Split-RI-J reference method, even for systems containing around 1000 atoms. While Split-RI-J remains the fastest approach for compact 3D molecules and linear systems with up to 300–400 atoms, RI-BUPO-J offers a scalable and competitive alternative for large or non-standard systems.

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Contributed Talk

A rigorous mixed electronic/classical DFT formalism for QM/MM systems

CT-14

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Combining classical density functional theory (cDFT) with quantum mechanics (QM) methods offers a computationally efficient alternative to traditional QM/molecular mechanics (MM) approaches for modeling mixed quantum-classical systems at finite temperatures. However, both QM/MM and QM/cDFT rely on somewhat ambiguous approximations.

In this presentation I will present our latest results on the exact theoretical framework that allows us to clarify the approximations involved in the QM/cDFT formulation and serves as a starting point for further development. We therefore establish a comprehensive density functional theory (DFT) framework for mixed quantum-classical systems within the canonical ensemble. A mean-field approximation is finally introduced in the context of solvation problems and we discuss its connection with several existing mixed cDFT-eDFT schemes.

INVITED TALK

Theoretical description of 4f and 5f complexes

IT-16

by Hélène Bolvin ^{1*,†}

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France*

The quantum chemical description of open-shell 4f (lanthanide) and 5f (actinide) complexes presents unique theoretical and computational challenges due to their complex electronic structures, strong electron correlation, and significant relativistic effects. There are many low-lying states, spin-orbit effects are important and essential and correlation effects must be taken into account. CAS based approaches are the cornerstone of the approaches for a correct description of absorption spectra and magnetic properties, as SO-CASPT2 or SO-NEVPT2

In this presentation, I will develop two examples where it is necessary to go beyond the SO-CASPT2 approach.

i) Absorption of lanthanide complexes.

While f-f transitions in lanthanide complexes are Laporte forbidden, some transitions in the non-centrosymmetric complexes, denoted hypersensitive, are strongly exalted and highly sensitive to changes in symmetry, polarizability, and coordination geometry of the ligands. While the SO-CASPT2 method manages to place the transition, one needs to add on the top of the CASSCF the CIS in order to render the oscillator strength of the transitions, as described by the dynamic coupling model.

ii) Ligands paramagnetic NMR of actinide complexes

The paramagnetic chemical shift is the part of the shift that is due to the presence of the paramagnetic center, in our case an actinide cation. This shift may be split into a dipolar term well described by SO-CASPT2, and a contact term, which needs a precise description of spin delocalization and polarization on the ligands, well captured by unrestricted DFT methods [1].

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Md. A. Islam, H. Bolvin in G. Aucar (Ed) 'NMR spectroscopic parameters: Theories and Models, Computational Codes and Calculations' Royal Society of Chemistry 2025

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INVITED TALK

Quantum Computing for Polaritonic Chemistry: *Which Platform Could Work Best?*

IT-17

Saad Yalouz

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Simulating *ab initio* polaritonic chemistry (*i.e.*, quantum chemistry in an optical cavity) on quantum computers presents a significant challenge, primarily due to the need for efficient encoding of strongly correlated hybrid “electron+photon” states within quantum circuits. Given that such problems involve both fermionic and bosonic degrees of freedom, it is natural to question whether conventional *qubit-based* approaches are optimal, or whether alternative (and potentially more exotic) quantum computing paradigms might offer more suitable solutions.

In this talk, I will discuss three strategies for encoding coupled “fermion+boson” systems across different quantum computing platforms. More precisely, I will consider platforms that employ distinct types of quantum information units, namely: *quBits*, *quDits*, and *quModes*. For each architecture, I will introduce dedicated encoding schemes and highlight their performance in describing a so-called *Light Induced Avoided Crossing*. The latter represents a characteristic spectral feature of polaritonic systems that is a direct signature of strong light-matter correlations.

POSTER PRESENTATION

Toward beyond-*GW* accuracy with Parquet theory for molecules

PP-01

by Antoine Marie ^{1*},[†], and Pierre-François Loos¹

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The amazing cost-to-accuracy ratio of *GW* theory has been both a blessing and a curse for the electronic structure community. Its cheap cost has made it the state-of-the-art method to compute ionization potentials of large molecular systems or extended systems [1,2]. However, for cases where one require more accurate prediction (or in cases where *GW* fails), a post-*GW* method with a larger computational cost but offering systematic improvement has been elusive so far [3]. This can be traced back to the fortuitous cancellation of error achieved by *GW*.

In this work, an alternative route to post-*GW* theory is investigated, namely the Parquet theory which implements self-consistency at the one-and two-particle level [4]. This comes with a larger computational cost but allows to treat every so-called correlation channels on an equal footing while *GW* emphasizes the importance of the particle-hole channel. For example, this has been shown to be important to go toward the strongly correlated regime of the Hubbard model. This work extends these studies on lattice models by implementing an approximate Parquet theory in typical quantum chemistry Gaussian basis sets. Its accuracy is assessed and compared to usual approximations such as *GW* and Coupled-Cluster.

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POSTER PRESENTATION

Correction basis method for double hybrid approximations in functional density theory

PP-02

by Aurore Znaïda[†] and Julien Toulouse¹

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Knowing the electronic structure of a system (atom, molecule or solid) allows to predict its chemical properties. Calculating the electronic structure of a system requires in principle to find the many-body wave function by solving the Schrödinger equation. Unfortunately, the Schrödinger equation is only solvable for simple cases, which explains the need of developing approximations or ways to bypass this equation to study more complicated cases. A way to bypass the Schrödinger equation is density-functional theory (DFT) [1], which consists in replacing the calculation of the many-body wave function by using density functionals, unlike wave-function methods which rely on direct approximations of the wave function [2]. The advantage of DFT over those direct wave-function methods is to reduce calculation costs. Nowadays, a popular family of approximations within DFT is given by the so-called double-hybrids, which combine a wave-function contribution and a density-functional contribution, and offer a balance between accuracy and calculation cost [3,4]. The wave-function contribution accounts for a fraction (depending on a chosen parameter) of the energy whereas the density-functional contribution accounts for the complementary fraction. However, since the wave-function contribution is calculated with a finite -rather than infinite- number of orbitals, a part of the energy is lost. This results in less accurate energies, especially for small orbital bases (basis with a small number of orbitals), which is called a slow convergence problem of the energy with respect to the size of the basis. This problem can be addressed by adding corrective terms, which are able to estimate the missing energy in a given orbital basis. In this work, two basis corrective terms, a basis-set correction for the correlation energy and a Kohn-Sham correction for the one-electron energy, are tested on small representative test sets of atomatization energies (AE6) and reaction barrier heights (BH6) [5], and their efficiency to improve the convergence for small basis is proven. Results are compared with a recent work using similar basis corrective terms [6].

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POSTER PRESENTATION

X-Ray Absorption meets Matrix Product States: excitation spectrum of impurity models via a MPS-based Lanczos algorithm

PP-03

by Coraline Letouzé^{1*}[†], Sebastian Paeckel², Guillaume Radtke¹ and Benjamin Lenz¹

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In strongly correlated materials like transition metal (TM) oxides, core-level spectroscopies such as X-ray Absorption Spectroscopy (XAS) are usually solved on a small cluster made of the valence and core states of the TM ion and its oxygen ligands. This cluster is then diagonalized exactly via the Lanczos algorithm. In the quest to extend this cluster model into an impurity model, beyond the capabilities of Exact Diagonalization, we apply the Lanczos algorithm on Matrix Product States (MPS). Compared to standard valence-only impurity models, the inclusion of core levels leads to more interacting orbitals connected by an intricate interaction network. In addition, the XAS spectrum requires resolving relatively high excitation energies (of around 20 eV), which are challenging to converge within the Lanczos algorithm.

In this poster, I will present our results on impurity models for simple TM oxides (NiO, MnO), with a focus on the numerical stability and convergence of the MPS-based Lanczos solver. I will also report on my attempt to implement the shift-and-invert Lanczos method.

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Toward Accurate van der Waals Modeling: A Comparative Study of Empirical and Physical Approaches Using *VMoPro* and *MoProViewer*

PP-04

by Mambatta Haritha[†], Benoît Guillot¹, and Christian Jelsch*¹

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Understanding molecular recognition, crystal packing, and biological processes including protein–ligand binding, protein folding, and macromolecular structure all depend on accurate modeling of non-covalent interactions. In this study, we introduce and evaluate two complementary van der Waals (vdW) models—empirical and physically grounded—for computing exchange-repulsion, dispersion, and total vdW interaction energies. A set of 21 atom-type-specific vdW parameters (σ , ε , δ , and γ) was derived via a least-squares optimization using the SciPy library and implemented in the *VMoPro* software. The empirical model yields highly accurate interaction energies, exhibiting a strong correlation ($R = 0.990$) with reference Symmetry-Adapted Perturbation Theory (SAPT) values from the extensive NENCI-2021 dataset¹ comprising 6,000 diverse molecular dimers. The physical model—implemented in *MoProViewer*²—utilizes electron density and transferred atomic polarizabilities³ from the ELMAM2 database to estimate exchange-repulsion and dispersion energies⁴. The vdW energies determined using the physical model exhibit a significant correlation, $R = 0.956$, with SAPT data, and a distance-dependent analysis showed that correlation improves with increasing intermolecular separation (0.80 to 1.10 Å). Together, these results demonstrate that the empirical *VMoPro* model, supported by optimized parameters, offers a computationally efficient and accurate alternative to high-level quantum mechanical methods. The physical model further emphasizes the significance of accurate electron density and polarizability parameters for correct vdW interaction estimation.

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POSTER PRESENTATION

Range-separated density functional theory for single-photon atomic ionization

PP-05

by J. van Gog¹, F. Zapata², and J. Toulouse¹

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Advancements in attosecond physics increasingly demand theoretical models to explain measurement outcomes. This project aims at deriving and implementing the linear-response Sternheimer equations for closed-shell atoms in order to investigate single-photon ionization by means of a B-spline based code written in Fortran. As an introduction to range-separated density functional theory, the locally range-separated hybrid version has been implemented as well. The results demonstrate accurate energy values and oscillator strengths for the Hartree-Fock method and the local-density approximation. Furthermore, the locally range-separated hybrid orbital energies align well with previous calculations. Finally, the time-dependent Hartree-Fock method offers significant improvements of the photoionization spectrum over the bare version. The time-dependent local-density approximation offers a smaller improvement with respect to its bare version; however, at high energies the correct behavior is reproduced.

Benchmark study of many-body methods for the prediction of band alignment at hetero-interfaces, using 1D Hubbard models

PP-06

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In a photovoltaic cell, a current is obtained by breaking photo-induced electron-hole pairs at a junction between an absorber and a transport layer. This separation is made possible by a proper offset of the electronic bands at the interface. Therefore, predicting this band offset with good precision is crucial for predicting the efficiency of the cell. Most many-body techniques however fail at reliably predicting the valence and conduction band offsets in agreement with experimental data [1]. In addition, discrepancies appear between the experimental values as well. Therefore, a benchmark study of the band alignment in various types of heterojunctions is needed. The approach presented in this talk is to start from the simplest model junction, the asymmetric Hubbard dimer, and study the range of validity of several many-body approximations in all possible regimes. This model has the great advantage to be exactly solvable, providing the exact addition/removal energies as a benchmark. In particular, results for exact Kohn-Sham DFT, Hartree-Fock and several GW flavors will be discussed. This study is then extended to an asymmetric Hubbard chain, to better capture physics of systems with interfaces relevant to photovoltaic applications.

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POSTER PRESENTATION

Complex Absorbing Potential Green's Function Methods for Resonances

PP-07

by Loris Burth^{1,†} and Pierre-Francois Loos^{1,*}

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The Complex Absorbing Potential (CAP) formalism has been successfully employed in various wavefunction-based methods to study electron resonance states, such as Configuration Interaction and Coupled Cluster theories [1-3]. In contrast, Green's function-based methods are widely used to compute ionization potentials and electron affinities but have not traditionally been applied to resonances.

We implement the CAP formalism within the *GW* approximation, enabling the description of electron resonance states in a Green's function framework. This approach entails a fully complex treatment of orbitals and quasiparticle energies in a non-Hermitian setting. We validate our implementation on prototypical systems such as N₂⁻ and CO⁻, demonstrating that it offers a fast and practical route to approximate both the lifetimes and positions of resonance states.

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POSTER PRESENTATION

Forces and phonons with advanced density functional theory methods PP-08

by Damian Contant*, Michele Casula, and Maria Hellgren*,†

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Knowing the forces exerted on the nuclei is important for determining equilibrium geometries and calculating vibrational modes. The accuracy achieved will, however, crucially depend on the level of description of the electron-electron interaction, which directly determines the potential energy surface of the nuclei. Methods based on the random phase approximation (RPA) are usually formulated within the DFT framework, in which the energy and density are obtained self-consistently under the action of a local Kohn-Sham potential [1]. The exchange correlation part of this potential is obtained by solving the so-called Optimized Effective Potential (OEP) equation [2]. At self-consistency, forces can be determined through the Hellmann-Feynman theorem. We have successfully implemented OEP forces within the Quantum ESPRESSO plane-wave code [3], finding forces with excellent numerical precision on different molecular and solid state systems [4]. We show that already the RPA, that includes the Hartree kernel only, systematically improves the description of geometries and vibrational frequencies, upon semi-local approximations in DFT. By including also the exchange kernel within RPAX we are able to achieve an accuracy comparable to CCSD(T).

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POSTER PRESENTATION

How to do *GW* for superconductors?

PP-09

by M. Rodríguez-Mayorga^{1,*†}, and P.-F. Loos^{1,*}

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In computational chemistry, the starting point for *ab-initio* simulations is, usually, the Hartree–Fock method. On top of this method, we have developed the concept of electronic correlation effects and the post-Hartree–Fock methods to account for these effects. Recently, many-body perturbation theory methods (e.g., *GW*, *BSE*, etc.) have crossed the border from the physics to the chemistry community; to become strong competitors in the search for cost-effective methods able to account for the electronic correlation effects and predict properties of materials (e.g., ionization potentials, electron affinities, spectra, etc.). For studying superconductivity, *ab-initio* simulations have relied on the Hartree–Fock–Bogoliubov method, which can be seen as an extension of the Hartree–Fock method where the number of particles is allowed to fluctuate. Unfortunately, being still mean-field method, the Hartree–Fock–Bogoliubov method misses some of the electronic correlation effects that can play a fundamental role in the description of superconductors. To account for these effects, we propose to incorporate the *GW* approximation for the study and design novel superconductors. In this poster, I will introduce the Hartree–Fock–Bogoliubov method and discuss our plan to incorporate the *GW* approximation in *ab-initio* simulations of superconductors.

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POSTER PRESENTATION

Calculation of first and second hyperpolarizabilities with (relativistic) Coupled-Cluster theory for sulfur-containing systems

PP-10

by Maxime LE¹, Loic Halbert¹, and Andre Severo Pereira Gomes¹

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Light-matter interactions provides insight about the system under study, and by considering both the linear and nonlinear responses we can gain complementary information on a system. Materials can be designed for their non-linear optical (NLO) properties, such as the first (β) and second (γ) hyperpolarizabilities [1,2]. These effects represent complex phenomena, since multiple photons are involved.

Unlike the case of light element molecules, simulations of NLO properties with accurate wavefunction-based methods for systems containing heavy elements (for which relativistic effects need to be taking into account) remains relatively unexplored. In this contribution we aim to start bridging this gap, by investigating the performance of the CCSD method to obtain the frequency-dependent γ of CS₂, a well-known benchmark for studying non-linear optics, and for which γ has recently been measured in the gas phase [2]. Relativistic and correlation effects are further investigated at the CCSD level for frequency-independent β and γ of XS (X = C-Pb) model systems.

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POSTER PRESENTATION

Excited states of the uniform electron gas

PP-11

by Pierre-François Loos^{1,*†}

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The uniform electron gas (UEG) [1] is a cornerstone of density-functional theory (DFT) and the foundation of the local-density approximation (LDA), one of the most successful approximations in DFT. In this poster, we extend the concept of UEG by introducing excited-state UEGs, systems characterized by a gap at the Fermi surface created by the excitation of electrons near the Fermi level [2]. We report closed-form expressions of the reduced kinetic and exchange energies of these excited-state UEGs as functions of the density and the gap. Additionally, we derive the leading term of the correlation energy in the high-density limit. By incorporating an additional variable representing the degree of excitation into the UEG paradigm, the present work introduces a new framework for constructing local and semi-local state-specific functionals for excited states [3].

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[†] Speaker

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V. Organization of the congress and financial support

V. Organizing committee

Séverine BONENBERGER

Thibaud ETIENNE

Jérémie MORERE

Julien TOULOUSE

V.2 Scientific committee

Lorenzo Ugo ANCARANI

Eric CANCÈS

Thomas DUGUET

Emmanuel FROMAGER

Emmanuel GINER

Pascal GRANGER

Maria HELLGREN

Pierre-François LOOS

Paola NAVA

Pina ROMANELLO

André SEVERO PEREIRA GOMES

Julien TOULOUSE

Morgane VACHER

V.3 Financial support

We would like to warmly thank the following departments for their generous financial support:

- The faculty of science and technology for lending us the amphitheater
- The CPM scientific pole of the university of Lorraine
- The C2MP PhD school of the university of Lorraine
- The laboratory of theoretical physics and chemistry (CNRS and university of Lorraine)
- The CNRS, through the NBODY research network
- The European Research Council (ERC) through the “European Union’s Horizon Europe” research and innovation program (Grant agreement No. 101163469)

T3

PÉRIODE VERTE
SEMAINE SCOLAIRE

DU LUNDI AU VENDREDI

HORAIRES EN SERVICE
À PARTIR DU 7 AVRIL 2025

DIRECTION VILLERS Campus Sciences

Séchamps Halle Certin	05:00	05:30	06:00	06:11	06:21	06:31	06:41	06:49
Essey Porte Verte	05:09	05:39	06:09	06:20	06:30	06:40	06:51	06:59
Essey Mouzimpré	05:14	05:44	06:14	06:25	06:35	06:45	06:57	07:05
Place des Vosges	05:27	05:57	06:27	06:38	06:48	06:58	07:12	07:20
Tour Thiers Gare	05:34	06:04	06:34	06:45	06:55	07:05	07:21	07:29
Provinces	05:44	06:14	06:45	06:56	07:06	07:17	07:38	07:46
Villers Mairie	05:49	06:19	06:50	07:01	07:11	07:22	07:45	07:53
Villers Campus Sciences	05:53	06:23	06:55	07:06	07:16	07:27	07:51	07:59
Séchamps Halle Certin	06:56	07:03						
Essey Porte Verte	07:06	07:13						
Essey Mouzimpré	07:12	07:19						
Place des Vosges	07:27	07:34						
Tour Thiers Gare	07:36	07:43						
Provinces	07:53	08:00						
Villers Mairie	08:00	08:07						
Villers Campus Sciences	08:06	08:13						
Séchamps Halle Certin								
Essey Porte Verte								
Essey Mouzimpré								
Place des Vosges								
Tour Thiers Gare								
Provinces								
Villers Mairie								
Villers Campus Sciences								

Villers Campus Sciences	05:00	05:30	06:00	06:11	06:21	06:31	06:41	06:49
Villers Mairie	05:05	05:35	06:05	06:16	06:26	06:36	06:46	06:54
Provinces	05:09	05:39	06:09	06:20	06:30	06:40	06:50	06:58
Saint-Léon	05:20	05:50	06:21	06:32	06:42	06:52	07:03	07:11
Place des Vosges	05:28	05:58	06:29	06:40	06:50	07:00	07:11	07:19
Essey Mouzimpré	05:39	06:09	06:40	06:51	07:01	07:13	07:24	07:32
Essey Porte Verte	05:45	06:15	06:47	06:58	07:08	07:20	07:31	07:39
Séchamps Halle Certin	05:54	06:24	06:56	07:07	07:17	07:29	07:41	07:49
Villers Campus Sciences	06:56	07:03						
Villers Mairie	07:01	07:08						
Provinces	07:05	07:12						
Saint-Léon	07:18	07:25						
Place des Vosges	07:26	07:35						
Essey Mouzimpré	07:40	07:50						
Essey Porte Verte	07:48	07:58						
Séchamps Halle Certin	08:00	08:10						
Villers Campus Sciences								
Villers Mairie								
Provinces								
Saint-Léon								
Place des Vosges								
Essey Mouzimpré								
Essey Porte Verte								
Séchamps Halle Certin								
Villers Campus Sciences	21:00	21:20	21:40	22:00	22:30	23:00	23:30	00:13
Villers Mairie	21:05	21:25	21:45	22:05	22:35	23:05	23:35	00:18
Provinces	21:08	21:28	21:48	22:08	22:38	23:08	23:38	00:21
Saint-Léon	21:20	21:40	22:00	22:20	22:50	23:20	23:50	00:33
Place des Vosges	21:28	21:48	22:08	22:28	22:58	23:28	23:58	00:41
Essey Mouzimpré	21:40	22:00	22:20	22:40	23:10	23:40	00:10	00:53
Essey Porte Verte	21:45	22:05	22:25	22:45	23:15	23:44	00:14	00:43
Séchamps Halle Certin	21:54	22:14	22:34	22:54	23:53	00:23	00:52	
Villers Campus Sciences								
Villers Mairie								
Provinces								
Saint-Léon								
Place des Vosges								
Essey Mouzimpré								
Essey Porte Verte								
Séchamps Halle Certin								

**CONSULTEZ
LES INFOS
TRAFFIC
EN TEMPS RÉEL**

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03 83 30 08 08

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DIRECTION SEICHAMPS Halle Certin

Seichamps Halle Certin	21:00	21:20	21:40	22:00	22:30	23:00	23:30	00:13
Essey Porte Verte	21:08	21:28	21:48	22:08	22:38	23:07	23:37	00:06
Essey Mouzimpré	21:13	21:33	21:53	22:13	22:43	23:12	23:42	00:11
Place des Vosges	21:25	21:45	22:05	22:25	22:55	23:24	23:54	00:23
Tour Thiers Gare	21:33	21:53	22:13	22:33	23:03	23:32	00:02	00:31
Provinces	21:45	22:05	22:25	22:45	23:15	23:44	00:14	00:43
Villers Mairie	21:50	22:10	22:30	22:50	23:20	23:49	00:19	00:48
Villers Campus Sciences	21:54	22:14	22:34	22:54	23:53	00:23	00:52	
Seichamps Halle Certin								
Essey Porte Verte								
Essey Mouzimpré								
Place des Vosges								
Tour Thiers Gare								
Provinces								
Saint-Léon								
Place des Vosges								
Essey Mouzimpré								
Essey Porte Verte								
Seichamps Halle Certin								

T1

PÉRIODE VERTE
DU LUNDI AU VENDREDI
(Y COMPRIS PENDANT LES VACANCES SCOLAIRES)

DU LUNDI AU VENDREDI
À PARTIR DU 5 AVRIL 2025

HORAIRES EN SERVICE

DIRECTION WANDŒUVRE Brabois - Hôpitaux

Essey Mouzimpré	04:00	04:15	04:30	04:45	05:00	05:10	05:20	05:30	05:40	06:00	06:10	06:20
Mairie de Saint-Max	04:09	04:24	04:39	04:54	05:09	05:19	05:29					
Point Central	04:17	04:32	04:47	05:02	05:17	05:27	05:37					
Gare - Saint-Léon	04:22	04:37	04:52	05:07	05:22	05:32	05:42					
Jean Jaurès	04:25	04:40	04:55	05:10	05:25	05:35	05:45					
Vélodrome - Callot	04:31	04:46	05:01	05:16	05:31	05:41	05:51					
Vandœuvre Brabois - Hôpitaux	04:41	04:56	05:11	05:26	05:41	05:51	06:01					

Essey Mouzimpré	21:10	21:25	21:40	21:55	22:10	22:25	22:40	22:55	00:10	00:25	00:40	00:55
Mairie de Saint-Max	21:18	21:33	21:48	22:03	22:18	22:33	22:48					
Point Central	21:26	21:41	21:56	22:11	22:26	22:41	22:56					
Gare - Saint-Léon	21:32	21:47	22:02	22:17	22:32	22:47	23:02					
Jean Jaurès	21:35	21:50	22:05	22:20	22:35	22:50	23:05					
Vélodrome - Callot	21:41	21:56	22:11	22:26	22:41	22:56	23:11					
Vandœuvre Brabois - Hôpitaux	21:51	22:06	22:21	22:36	22:51	23:06	23:21					

Vandœuvre Brabois - Hôpitaux	04:50	05:05	05:20	05:35	05:50	06:00	06:10	06:20	06:35	06:50	06:59	07:14
Vélodrome - Callot	04:58	05:13	05:28	05:43	05:58	06:08	06:18	06:28				
Jean Jaurès	05:04	05:19	05:34	05:49	06:04	06:14	06:24	06:35				
Gare - Saint-Léon	05:08	05:23	05:38	05:53	06:08	06:18	06:28	06:39				
Point Central	05:12	05:27	05:42	05:57	06:12	06:22	06:32	06:43				
Mairie de Saint-Max	05:20	05:35	05:50	06:05	06:20	06:30	06:40	06:51				
Essey Mouzimpré	05:27	05:42	05:57	06:12	06:27	06:37	06:47	06:59				

DIRECTION ESSEY Mouzimpré

Vandœuvre Brabois - Hôpitaux	22:15	22:30	22:45	23:00	23:15	23:30	23:45	23:50	00:00	00:15	00:30	00:45
Vélodrome - Callot	22:33	22:38	22:53	23:08	23:23	23:38	23:53	23:58				
Jean Jaurès	22:39	22:45	23:00	23:15	23:30	23:45	00:00	00:15				
Gare - Saint-Léon	22:44	22:49	23:04	23:19	23:34	23:49	00:04	00:19				
Point Central	22:48	22:53	23:08	23:23	23:38	23:53	00:08	00:23				
Mairie de Saint-Max	22:54	23:09	23:24	23:39	23:54	00:09	00:24	00:39				
Essey Mouzimpré	22:54	23:09	23:24	23:39	23:54	00:09	00:24	00:39				

HORAIRES EN TEMPS RÉEL

PROCHAINS PASSAGES :

Envoyez le code arrêt au **07 55 54 14 00** (coût d'envoi d'un SMS) et scannez le QR Code. Ces informations sont présentes à chaque arrêt sur les fiches horaires affichées.



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**CONSULTEZ
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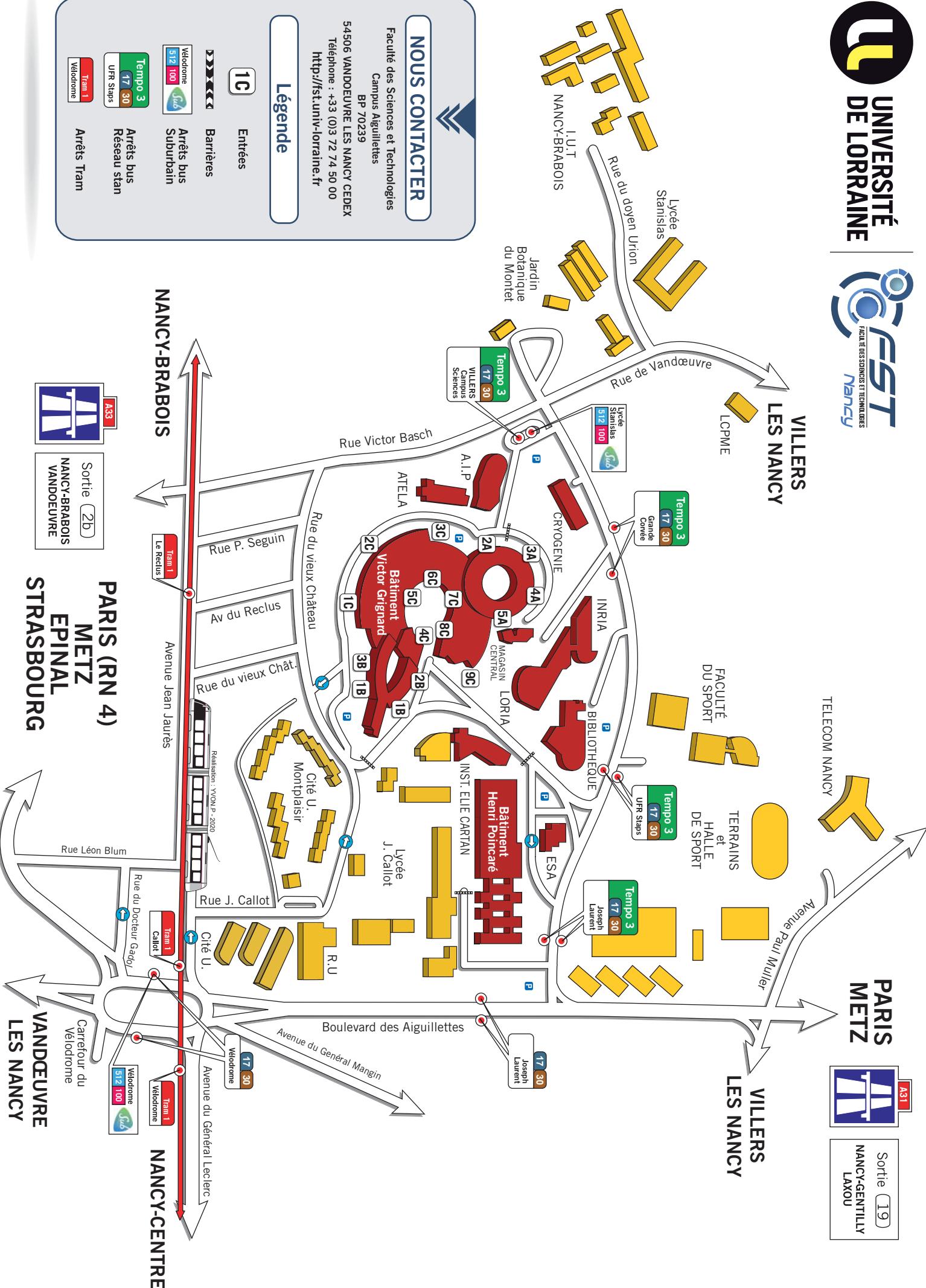


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BP 70239
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Téléphone : +33 (0)3 72 74 50 00
<http://fst.univ-lorraine.fr>

Légende

- 1C** Entrées
- Barrières
- Arrêts bus Suburbain
- Arrêts Réseau stan
- Arrêts Tram
- Tempo 3** 17 30 UFR Staps
- Tram 1** Vélodrome
- A33** Sortie 2b NANCY-BRABOIS VANDOEUVRE
- Tempo 3** 17 30 UFR Staps
- Tram 1** Vélodrome
- Tempo 3** 17 30 UFR Staps
- Tram 1** Vélodrome
- Tempo 3** 17 30 UFR Staps
- Tram 1** Vélodrome



Bâtiment Victor Grignard

3ème niveau - Salles VG

- █ Services informatique et techniques
- █ Amphithéâtres VG1 à VG8
- █ Salles VG 301 à VG 324
- █ Salles VG3 TP 1 à VG3 TP 48
- █ Associations
- █ Toilettes
- █ Espace vert (extérieur)

