13th OpenMolcas Developers' Workshop

Schedule

Institute for Advanced Study,
Technical University of Munich,
June 11th-13th 2025

Schedule: Wed, June 11th

9:20	**Opening**	
9:30	**Reinhard Kienberger**	Attosecond science – from the beginning to measuring electron dynamics in molecules, solids and layered systems
10:20	**Jesús González-Vázquez**	Time-resolved ionization close to the threshold: RABBIT N2 with XCHEM
10:45	**Xiaoyu Mi**	Magnetic X-ray Scattering as a Probe of Ultrafast Molecular Spin-State Dynamics: An Ab Initio Theory.
11:10	**Michael Coates**	Ultrafast 3d metal L-edge spectroscopy studied by molecular dynamics and quantum chemistry
Coffee break (11:35 - 12:00)		
12:00	**Felix Plasser** (Online)	Multireference computations on π-conjugated diradicals
12:25	**Andy Kaiser**	Exchange Effects in Molecular Aggregates
12:50	**Luca De Vico**	Towards chromophore aggregates' exciton design, the multiconfigurational way
Lunch break (13:15 - 14:30)		
14:30	**Christian Schilling**	Quantum Information Perspective on the Ground State Problem: What is Electron Correlation?
15:20	**Stefano Battaglia**	Development of QD-CASPT2 variants based on DMRG reference states
15:45	**Kalman Szenes, Valentin Barandun**	QCMaquis 4.0: Multi-Purpose Electronic, Vibrational, and Vibronic Structure and Dynamics Calculations with the Density Matrix Renormalization Group
Coffee break (16:25 - 16:50)		
16:50	**Flash Presentation**	
17:00	**Poster session**	

Schedule: Thu, June 12th

9:30	**Piero Altoe**	Accelerating Quantum Chemistry with NVIDIA Technologies
10:20	**Valera Veryazov**	OpenMolcas and Education in Quantum Chemistry
10:45	**Andrew Sand**	Characterization of electron transport in molecular devices and wires using active space methods
Coffee break (11:10 - 11:40)		
11:40	**George Booth** (Online)	Interpolating wave functions to accelerate photochemical dynamics
12:30	**Imaad Ansari**	Room-temperature quantum tunnelling at singularities drive enormous reaction speed-ups
Lunch break (12:55- 14:00)		
14:00	**Davide Avagliano**	Ab Initio Multiple Spawning Nonadiabatic Dynamics with OpenMolcas
14:25	**Dilara Farkhutdinova**	Understanding the Excited States of an Iron(III) NHC Complex: Insights from Multiconfigurational Methods
14:50	**Thais Scott**	Characterizing Photoredox Active Transition Metal Catalysts with Extended Active-Space Wave Functions from Density Matrix Renormalization Group
15:15	**Discussion (until ca. 16:00)**	
19:00	**Dinner**	

Schedule: Fri, June 13th

09:30	**Alessandro Loreti**	A novel algorithm that couples Quantum Dynamics with Molecular Mechanics: study on the excitation energy transfer process of NADH solvated water
09:55	**Thies Romig**	Ultrafast non-adiabatic dynamics with multi-configuration Ehrenfest method
10:20	**Francesco Segatta**	Time-resolved Spectroscopy with OpenMolcas: from quantum chemistry (through COBRAMM) to spectroscopy & insight
10:45	**Mihael Erakovic**	Tunneling splitting in benzoic acid dimers from multi-level Jacobi field instanton theory
Coffee break (11:10 - 11:40)		
11:40	**Arta Safari**	Recent Developments in Stochastic Complete Active Space Second-Order Perturbation Theory
12:05	**Luca Bonfirraro**	Stochastic-SplitGAS: A Multi-Reference Perturbation Theory Based on the Stocastic Imaginary-Time Evolution of Effective Hamiltonians
12:30	**Closing**	

Instructions for participants:

Online participation:

All the talks and the presentations will be streamed via a Zoom's call. To follow the workshop, join the shared room with your full name at the link:

https://tum-conf.zoom-x.de/j/69409751416?pwd=PDaYJaUHdJrss9coqAag2IyWpUX7kD.1

Meeting-ID: 694 0975 1416
Password: 749515

To give a talk, the organizers will give the right to present the screen to the upcoming presenter.

Poster presentation:

Wednesday at 16:50, there will be a flash presentation of each poster contribution. Each presenter will have a maximum of 2 minutes to introduce his/her poster, following the order given in the next page.

Subsequently, there will be a dedicated time for questions to the online posters. The organizers will share Zoom breakout sessions where the online posters can be discussed individually.

Finally, the in-person posters can be discussed at the standings around the meeting room.

Flash presentations:

1.	**Daniel Roca-Sanjuán (Online)**	Free energy determinations with free energy perturbation theory and OpenMolcas
2.	**David Francisco Macias Pinilla (Online)**	Improving Photoabsorption Cross-Section Predictions for Atmospheric Compounds via Anharmonic Corrections in Nuclear Ensembles
3.	**Lorenz Grünewald (Online)**	Refining Initial Condition Preparation for Surface Hopping by Including Explicit Laser Pulses
4.	**Lea Ibele**	Different Flavours of CASPT2 for Nonadiabatic Dynamics
5.	**Patrick Staschick**	Dyson-density approach to charge-transfer excitons
6.	**Mateja Hrast**	Ab-initio Auger spectrum of the ultrafast dissociating 2p−1 3/2 σ⋆ resonance in HCl
7.	**Pang Yu**	Molecular Descriptors for High-Throughput Virtual Screening of Fluorescence Emitters with Inverted Singlet-Triplet Energy Gaps
8.	**Giacomo Bassi**	Highly-Excited Electronic States with Density Matrix Renormalization Group (DMRG) via Core-Valence Separated Hamiltonian

Information about the campus:

Event Location and Accessibility:

The event will take place at the Institute of Advanced Studies (IAS) on TUM's Garching campus.

The venue is easily accessible from the city center using Munich's public transportation system via the U6 line. Additionally, buses are available to connect with nearby towns, and with the S-Bahn for the airport.

Lunch Options:

While lunches are not provided by the organizers, there are several dining options available on campus:

- **"Crazy Bean"** located inside the IAS building
- Food trucks and small restaurants at the **Galileo building**
- **"Gate-kitchen"**, just a few minutes' walk west of the IAS
- Food trucks and a bakery situated in front of the **campus' main bus station**

You can find more information about dining options on this page (in German): https://webarchiv.typo3.tum.de/TUM/fg/gastronomie-am-campus/index.html

Additional Resources:

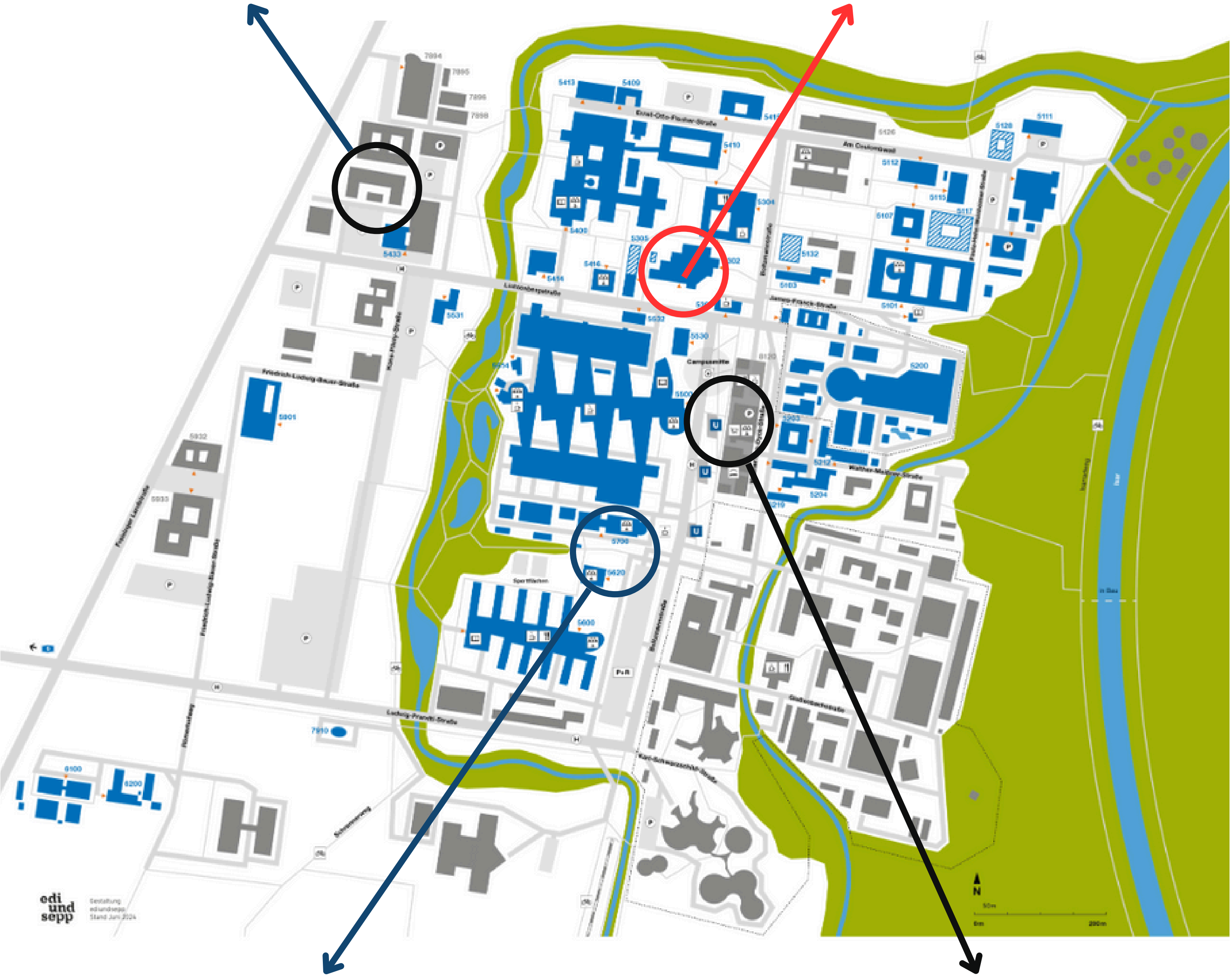
For more information about the venue and the city of Munich, you can visit the following websites:

- TUM's Garching campus: (https://www.tum.de/en/about-tum/locations/garching)
- IAS's webpage: (https://www.ias.tum.de/ias/start/)
- Munich City Hall portal: (https://www.muenchen.de/en/tourism)

Campus map:

Gate-kitchen

IAS building (Event location)



Bakery and food trucks

U-bahn station;
Galileo building

Dinner:

Dinner will take place at the Wirtshaus am Bavariapark on June 12 at 7:00 PM in the Bavariasaal.

Address: Theresienhöhe 15, 80339 München

The venue is centrally located and well connected to Munich’s public transport network. For example, take U6 from Garching-Forschungszentrum (direction Klinikum Großhadern). At Sendlinger Tor, transfer to the U4 or U5 (direction Westendstraße). Get off at Schwanthalerhöhe (1 stop). From Schwanthalerhöhe station, it’s about a 5-minute walk to the venue at Theresienhöhe 15.

Invited talk

Attosecond science – from the beginning to measuring electron dynamics in molecules, solids and layered systems

Reinhard Kienberger

School of Natural Sciences, E11, Technische Universität München, James Franck Straße, 85748 Garching, reinhard.kienberger@tum.de,

The generation and measurement of single isolated attosecond pulses in the extreme ultraviolet (XUV) at the beginning of this century has recently been awarded with the Nobel Prize in Physics [1]. This talk will give a historic review since the beginning of attosecond science and its impact on the understanding of electronic processes on the attosecond timescale.

A pump/probe technique, "attosecond streaking" [2], was used to investigate electron dynamics on surfaces and layered systems with unprecedented resolution. Photoelectrons generated by laser based attosecond extreme ultraviolet pulses (XUV), are exposed to a dressing electric field from well synchronized few-cycle infrared (IR) laser pulses. The energy shift experienced by the photoelectrons by the dressing field is dependent on the delay between the XUV pulse and the dressing field and makes it possible to measure the respective delay in photoemission between electrons of different type (core electrons vs. conduction band electrons). The information gained in such experiments on tungsten [3] triggered many theoretical activities leading to different explanations on the physical reason of the delay. Attosecond streaking experiments have been performed on different solids [4,5], layered structures and liquids, resulting in different delays – also depending on the excitation photon energy. These measurements lead to a stepwise increase of the understanding of different physical effects contributing to the timing of photoemission. In this presentation, an overview on the different physical contributions to attosecond time delays in photoemission will be given. The "absolute" time delay, i.e. the delay between the instant of ionization and the emission of a photoelectron will be discussed and latest measurements will be presented.

[1] M. Hentschel*, R. Kienberger* et al., Nature, 414, (2001)
[1] R. Kienberger et al., Nature 427, 817 (2004)
[2] A. Cavalieri et al., Nature 449, 1029 (2009)
[3] S. Neppl et al., Nature 517, 342 (2015)
[4] M. Ossiander et al., Nature 561, 374 (2018)

Contr. talk

Time-resolved ionization close to the threshold: RABBIT N_2 with XCHEM

Jesús González-Vázquez[1,2], Vicent J. Borràs[1], Luca Argenti[3] and Fernando Martín[1,4,5]

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The theoretical description of observables in attosecond pump-probe experiments requires a good representation of the ionization continuum. For poly-electronic molecules, however, this is still a challenge, due to the complicated short-range structure of correlated electronic wave functions. Whereas quantum chemistry packages designed to compute bound electronic molecular states are well established, comparable tools for the continuum are not widely available yet. To tackle this problem, we have developed a new approach [1] that, by means of a hybrid Gaussian-B-spline basis [2], interfaces existing multi-reference quantum chemistry packages (in particular using OpenMOLCAS [3]) with close-coupling scattering methods. In this talk, we will describe the ingredients of the method, already implemented in the XCHEM code, and illustrate its focusing on the N_2 molecule [4], including time-resolved simulations of its RABBIT spectrum [5].

References:

[1] C. Marante, M. Klinker, I. Corral, J. González-Vázquez, L. Argenti, and F. Martín, J. Chem. Theory Comput. **13**, 499 (2017).
[2] C. Marante, L. Argenti, and F. Martín, Phys. Rev. A **90**, 012506 (2014).
[3] F. Aquilante et al., J. Chem. Phys. **152**, 214117 (2020).
[4] M. Klinker, C. Marante, L. Argenti, J. González-Vázquez, and F. Martin, J. Phys. Chem. Lett. **9**, 756 (2018).
[5] V. J. Borràs, J. González-Vázquez, L. Argenti, and F. Martín, Sci. Adv. **9**, eade3855 (2023).

Contr.
talk

Magnetic X-ray Scattering as a Probe of Ultrafast Molecular Spin-State Dynamics: An Ab Initio Theory

Xiaoyu Mi[1], Ming Zhang[1], Linfeng Zhang[1], Leshi Zhao[1], Zhou Liang[1], Renxuan Peng[1], Zhaoheng Guo[2], Chengyin Wu[1,3,4], Sergey I. Bokarev[5,6] and Zheng Li[1,3,4]

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[3]*Collaborative Innovation Center of Extreme Optics, Shanxi University, Taiyuan, Shanxi 030006, China*
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With the advancement of the high harmonic generation and x-ray free-electron lasers (XFELs) to the attosecond domain, the studies of the ultrafast electron and spin dynamics became possible. Yet, the methods for efficient control and the measurement of the quantum state are to be further developed. We propose using magnetic x-ray scattering (MXS) for resolving the molecular spin-state dynamics and establish a complete protocol to simulate MXS diffraction patterns in molecules with ab initio quantum chemistry based on the multiconfigurational method. The performance of the method is demonstrated for the simulation of the spin-flip dynamics in $TiCl_4$ molecules [1].

In the $TiCl_4$ spin-flip dynamics initiated by an ultrashort x-ray pulse, the spin-orbit coupling strength is enough to trigger the crossover between electronic singlets and triplets, which is not necessarily connected to nuclear motion. The consistent variation of the electron population and the circular dichroic patterns show the capability of MXS to detect the spin-state dynamics in real time quantitatively. We also conclude that the spatial shape and extent of the spin density can also be inferred by analyzing diffraction patterns for randomly oriented and aligned molecules.

Our theoretical work and simulation [2] also show that in CH_2OH photodissociation process, the dissociation rates and the evolution of the electronic density of molecules caused by the effective force from Berry curvature can be observed with ultrafast x-ray diffraction using free electron lasers.

References

[1] **X. Mi**, M. Zhang et al., Non-Resonant Magnetic X-ray Scattering as a Probe of Ultrafast Molecular Spin-State Dynamics: An Ab Initio Theory. J. Chem. Theory Comput., 21(2), 549-559 (2025)

[2] M. Zhang, **X. Mi** et al., Observing a Berry Curvature Effect in CH_2OH Photodissociation via Molecular Dynamics Simulations. Phys. Rev. B, 109, 184304 (2024).

Contr.
talk

Ultrafast 3d metal L-edge spectroscopy studied by molecular dynamics and quantum chemistry

Michael R. Coates[a†], Hampus Wikmark[b], Raphael M. Jay[b], Ambar Banerjee[a,b], Philippe Wernet[b], Michael Odelius[a]

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Transition metal carbonyls have been central to the study of organometallic photochemistry. Upon ultraviolet excitation, these complexes often undergo carbonyl dissociation[1] generating short-lived, reactive intermediates that can bind a molecule from the surrounding solvent.[2] Vibrational cooling timescales and the complex free energy surface of the electronic ground state dictate the formation of transient species and photoproducts.

In this work, we use *ab initio* molecular dynamics (AIMD) simulations to simulate a benchmark system: $^{1}\mathrm{Fe(CO)}_5$ solvated in ethanol and the solvated photoproducts $^{1}\mathrm{Fe(CO)}_4$ and $^{3}\mathrm{Fe(CO)}_4$ to assess the solvation and stability of the reactants and thermally equilibrated photoproducts.[3] We show that molecular orbital insights of the equilibrated photoproducts have clear spectral signals that correlate to shifts in the soft X-ray iron L-edge spectra.[4] We calculate the Fe L-edge spectra based on an underlying restricted active space self-consistent field (RASSCF) wavefunction in OpenMolcas. We extend this approach to probe a photodissociated $\mathrm{Cr(CO)}_6$ in octane[5] where the same spectral trends are observed.

[1] Turner *et al. Chem. Soc. Rev.*, **2022**, *51*, 5300-5329
[2] Banerjee *et al. Nat. Comm.*, **2022**, *13*, 1337
[3] Coates *et al. Inorg Chem*, **2024**, *63*, 10634−10647
[4] Wikmark *et al. Unpublished*, **2023**
[5] Jay *et al. J. Am. Chem. Soc.*, **2024,** *146*, 14000−14011

Contr. talk

Multireference computations on π-conjugated diradicals

Felix Plasser, Loughborough University, Loughborough, LE11 3TU, UK.

π-conjugated radicals, based on the tris(2,4,6-trichlorophenyl)methyl (TTM) motif, have emerged as new interesting options for optoelectronic applications. In particular, TTM-based di- and polyradicals possess fascinating electronic structure properties with states that are neither present in monoradicals nor in closed shell systems. It is the purpose of this talk to provide a phenomenological analysis of the excited states of diradicals and to present a discussion of practical computational aspects. It will be of particular interest to combine the two, i.e., how can we bridge between simple models and high-level computations?

This talk will first address some basic ideas on the states present in diradicals [1]. Here, it will be of interest to discuss how the WFA module of OpenMolcas [2] can be effectively used to reconstruct the different types of states present. It will also be interesting to highlight the challenges of CASSCF to describe the zwitterionic states involved [3] and suggest a solution.

In the second part of this talk, we discuss the use of OpenMolcas to explain the unexpected absorption and luminescence properties of a cyclopentadithiophene bridged tris(2,4,6-trichlorophenyl)methyl (TTM) diradical [4], highlighting how even complex large systems can be efficiently treated using the RICD method. The calculations show that the lowest energy absorption and emission of this system is due to a state of zwitterionic character (Fig. 1).

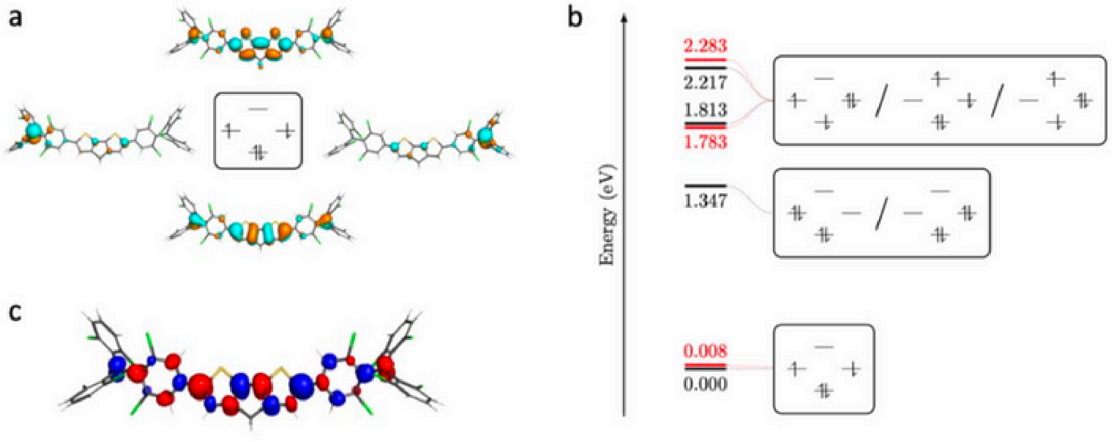

Figure 1: Excited states of a TTM-based π-conjugated diradical.

References

1. L. Matasović, H. Bronstein, R. H. Friend, F. Plasser. *Faraday Disc.* **2024**, *254*, 107.
2. F. Plasser, S. A. Mewes, A. Dreuw, L. González. *JCTC*, **2017**, *14*, 5343.
3. S. A. do Monte, et al. *JPCA*, **2023**, *127*, 9842.
4. C. Yu et al. *Sci. Adv.* **2024**, *10*, DOI: 10.1126/sciadv.ado3476.

Contr. talk

Exchange Effects in Molecular Aggregates

Andy Kaiser[a,b]

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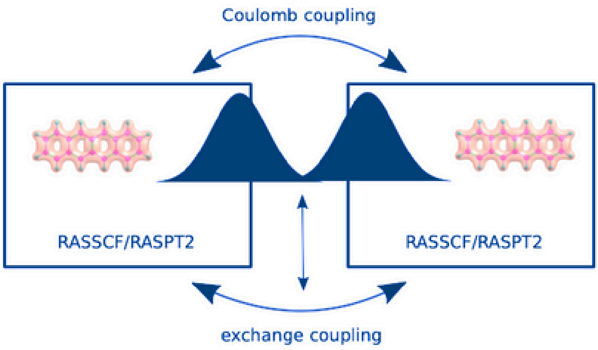

Understanding the photophysics of molecular aggregates is essential for designing advanced materials and devices across scientific disciplines. Accurate insight into their electronic structure is key, yet common approaches like (TD)DFT struggle with systems dominated by multiconfigurational effects, double excitations, and Rydberg states. In such cases, multi-configurational wavefunction-based methods are required, though their computational cost limits their use for larger aggregates. To overcome this, we employ the Frenkel exciton ansatz, enabling the treatment of dimers beyond the reach of supermolecule calculations. We present an OpenMolcas implementation that includes Coulomb interactions beyond the dipole approximation and is extended by the exchange to describe processes such as Dexter energy transfer, charge transfer, and singlet fission. Importantly, the exchange is computed by antisymmetrizing the product wave function, leading to terms beyond classical exchange that structurally resemble first-order symmetry-adapted perturbation theory (SAPT) corrections. As a perspective, we are developing a Dyson orbital-based method for addressing charge transfer states and an approach to model interactions between systems of different spin multiplicities.

Towards chromophore aggregates' exciton design, the multiconfigurational way

Razan E. Daoud,[1] Carlo Burresi,[1] Silvia Punis,[1] Giuseppe Mastrangeli,[1]
Emanuela Cetrullo,[2] Roberto Cacciari,[3] and Luca De Vico[1*]

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2 – Università degli Studi di Pisa, Dipartimento di Chimica e Chimica Industriale, via Giuseppe Moruzzi 13, 56124 Pisa, Italy

3 – Università degli Studi di Padova, Dipartimento di Scienze Chimiche, via Francesco Marzolo, 1, 35131 Padova, Italy

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In this talk, I will introduce our current work on computing excitonic properties and behaviour of chromophore aggregates, based on underlying multiconfigurational energetics. This work takes advantage of the possibility of computing Frenkel's excitonic couplings for homo- and hetero-dimers based on the monomers' wave functions and molecular transition densities computed at any flavour of multistate, multiconfigurational second order perturbation theory. [1] Besides, OpenMolcas allows rigidly roto-translating molecules and their optimized molecular orbitals, granting infinite dimers relative conformations at a comparatively very low computational cost. [2]

Building on our recent work on dimeric aggregates of bacteriochlorophyll derivatives, [3] I will present the predicted changes in a dozen-strong monomer aggregate test cases. Furthermore, following our previous studies on simulating the 27-bacteriochlorophyll-containing light-harvesting complex 2, [4] I will explore how relative pitch rotations may influence the overall simulated spectra.

Finally, I will present our current work on aggregates of cyanine-derived molecules. [5] After a first test run on a simple dimer, I will illustrate our attempt at reproducing the absorption spectra of self-assembled, halogen-substituted cyanine-based nanotubes. A 90-monomer aggregate was tried, representing a hopefully significant part of a nanotube.

[1] A. Kaiser, R. E. Daoud, F. Aquilante, O. Kühn, L. De Vico, S. I. Bokarev "A Multiconfigurational Wave Function Implementation of the Frenkel Exciton Model for Molecular Aggregates" J. Chem. Theory Comp. 2023, 19 (10), 2918-2928

[2] G. Li Manni et al. "The OpenMolcas *Web*: A Community-Driven Approach to Advancing Computational Chemistry" J. Chem. Theory Comp. 2023, 19 (20), 6933-6991

[3] R. E. Daoud, E. Cetrullo, L. De Vico "Tunable Spectral Properties and Excitonic Couplings of Bacteriochlorophyll-like Dimer Aggregates" ChemRxiv. 2025; DOI: 10.26434/chemrxiv-2025-37fb2

[4] R. Cacciari, R. E. Daoud, F. Aquilante, T. Hansen, L. De Vico "A Completely Multiconfigurational Description of LH2 Excitonic Couplings" Manuscript in preparation

[5] R. E. Daoud, C. Burresi, S. Punis, G. Mastrangeli, L. De Vico "Cyanine-based Nanotubes and Assemblies: a Multiconfigurational, Excitonic Description" Manuscript in preparation

Invited talk

Quantum Information Perspective on the Ground State Problem: What is Electron Correlation?

Christian Schilling

Arnold Sommerfeld Centre for Theoretical Physics, LMU Munich

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 electrons 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 and correlation inapplicable to electron systems in first quantization. However, in second quantization, where the focus shifts from particles to the inherently distinguishable orbitals, these concepts become well-defined. We then systematically apply this perspective to quantum chemistry. In particular, we show that it provides a deeper understanding of chemical bonding. Furthermore, we propose a systematic approach to enhancing wave function methods for strongly correlated electron systems, relevant to both classical and quantum computing. Altogether, these insights highlight the deep connection between quantum information and quantum chemistry, demonstrating fruitful synergies that can foster the second quantum revolution and lead to advances in electronic structure theory.

[1] L.Ding, C.Schilling, J. Chem. Theory Comput. 16, 7, 4159 (2020)

[2] L.Ding, S.Mardazad, S.Das, S.Szalay, U.Schollwoeck, Z.Zimboras, C.Schilling, J. Chem. Theory Comput. 17, 1, 79 (2021)

[3] L.Ding, S.Knecht, Z.Zimborás, C.Schilling, Quantum Sci. Technol. 8, 1, 015015 (2023)

[4] L.Ding, G.Duennweber, C.Schilling, Quantum Sci. Technol. 9, 1, 015005 (2023)

[5] L.Ding, S.Knecht, C.Schilling, J. Phys. Chem. Lett. 14, 11022 (2023)

[6] K.Liao, L.Ding, C.Schilling, J. Phys. Chem. Lett. 15, 6782 (2024)

[7] D.Aliverti-Piuri, K.Chatterjee, L.Ding, K.Liao, J.Liebert, C.Schilling, Faraday Discuss. 254, 76 (2024)

Development of QD-CASPT2 variants based on DMRG reference states

Kalman Szenes[1], Stefano Battaglia[2], and Markus Reiher[1]

[1] Department of Chemistry and Applied Biosciences, ETH Zurich, CH-8093 Zurich, Switzerland
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The density matrix renormalization group (DMRG) approach is a powerful method for obtaining accurate wave functions of strongly correlated systems [1, 2]. While it enables the calculation of ground and excited states with large active spaces beyond what is feasible with the complete active space self-consistent field (CASSCF), DMRG only captures static electron correlation without accounting for dynamic correlation effects. To address this limitation, the quasi-degenerate extensions of the complete active space second-order perturbation theory (QD-CASPT2) [3–5] provide a robust approach for incorporating dynamic correlation effects that also includes feedback to the underlying reference wave function. In this work, we present the integration of DMRG with QD-CASPT2 methods, enabling the calculation of dynamic correlation effects on top of a DMRG reference wave function. This combination facilitates the treatment of excited states with large active spaces that would otherwise be computationally intractable with traditional CASSCF approaches. In this presentation, we will discuss the current implementation status in OpenMolcas, powered by the QCMaquis program for DMRG calculations [6], and demonstrate preliminary results. Our work builds upon significant recent developments in OpenMolcas that have enhanced the CASPT2 module, allowing us to capitalize on these advancements for more accurate quantum chemical calculations.

[1] K. H. Marti and M. Reiher, "The Density Matrix Renormalization Group Algorithm in Quantum Chemistry", Zeitschrift für Phys. Chemie **224**, 583–599 (2010) `10.1524/zpch.2010.6125`.
[2] A. Baiardi and M. Reiher, "The density matrix renormalization group in chemistry and molecular physics: Recent developments and new challenges", J. Chem. Phys. **152**, 040903 (2020) `10.1063/1.5129672`.
[3] J. Finley, P.-Å. Malmqvist, B. O. Roos, and L. Serrano-Andrés, "The multi-state CASPT2 method", Chem. Phys. Lett. **288**, 299–306 (1998) `10.1016/S0009-2614(98)00252-8`.
[4] T. Shiozaki, W. Győrffy, P. Celani, and H.-J. Werner, "Communication: Extended multi-state complete active space second-order perturbation theory: Energy and nuclear gradients", J. Chem. Phys. **135**, 081106 (2011) `10.1063/1.3633329`.
[5] S. Battaglia and R. Lindh, "Extended Dynamically Weighted CASPT2: The Best of Two Worlds", J. Chem. Theory Comput. **16**, 1555–1567 (2020) `10.1021/acs.jctc.9b01129`.
[6] K. Szenes, N. Glaser, M. Erakovic, V. Barandun, M. Mörchen, R. Feldmann, S. Battaglia, A. Baiardi, and M. Reiher, *QCMaquis 4.0: Multi-Purpose Electronic, Vibrational, and Vibronic Structure and Dynamics Calculations with the Density Matrix Renormalization Group*, version 1, `10.48550/arXiv.2505.01405`, pre-published.

Contr. talk

QCMaquis 4.0: Multi-Purpose Electronic, Vibrational, and Vibronic Structure and Dynamics Calculations with the Density Matrix Renormalization Group[1]

Kalman Szenes[†], Nina Glaser[†], Mihael Erakovic[†], Valentin Barandun[†], Maximilian Mörchen[†], Robin Feldmann[†], Stefano Battaglia[‡], Alberto Baiardi[†], and Markus Reiher[†]

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QCMaquis is a quantum chemistry software package for general molecular structure calculations in a matrix product state/matrix product operator formalism of the density matrix renormalization group (DMRG). It supports a wide range of features for electronic structure, multi-component (pre-Born–Oppenheimer), anharmonic vibrational structure, and vibronic calculations. In addition to the ground and excited state solvers, QCMaquis allows for time propagation of matrix product states based on the tangent-space formulation of time-dependent DMRG. The latest developments include extending the interface to OpenMolcas to support complete active space second-order perturbation theory (CASPT2) calculations using a DMRG reference wavefunction, transcorrelated electronic structure theory, recent vibrational and vibronic models, and a convenient Python wrapper, facilitating the interface with external libraries. In this talk, we will give an overview of the new features in this major release of our QCMaquis program.

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Invited talk

Accelerating Quantum Chemistry with NVIDIA Technologies

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We believe that the urge to use Artificial Intelligence (AI) in the domain of computational chemistry is higher than ever and very much understandably so. However, training AI models for that purpose relies strongly on datasets that are large and of the highest possible accuracy. Generating those datasets in-turn needs efficiently implemented methods of quantum chemistry and GPUs have demonstrated their merit in accelerating scientific computing countless times and can bring down calculation times from years to months or even less; yet they have remained underutilized in quantum chemistry.

While a plethora of methods are available in quantum chemistry, those that offer highest accuracy go along with high computational cost and scaling. Considering AI training, this underlines the need of reusable highly optimized libraries that make best use of the available hardware resources. At the same time, domain experts should be empowered to focus on scientific research and not on refactoring tried-and-true code when hardware requirements change.

This presentation will give an overview of NVIDIA's hardware and software platform, how the various components can be leveraged in quantum chemistry acceleration and how they are used today in terms of practical examples. We will include an outlook on the software roadmap, some recent work to make development and maintenance of codes for GPU-accelerated quantum-chemistry even more accessible in the future and present our perspective on the role of platform providers in the quantum chemistry community.

OpenMolcas and Education in Quantum Chemistry

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Since its foundation, the motto of Molcas has been "software package developed by scientists for scientists." The growing OpenMolcas community demonstrates its widespread use in scientific research. However, apart from a few PhD studies - mostly supervised by OpenMolcas developers - its use in education remains scarce.

At the master's level education in quantum chemistry, programs such as Gaussian and Orca dominate. The challenge is not only the lack of graphical user interfaces but also deeper issues related to input structure, code organization, computed properties, and output interpretation. These observations are based on personal experience using OpenMolcas in workshops [1] and regular courses for master's and PhD students [2].

This talk will analyze the challenges of using OpenMolcas in education and propose possible improvements to make it more accessible for students.

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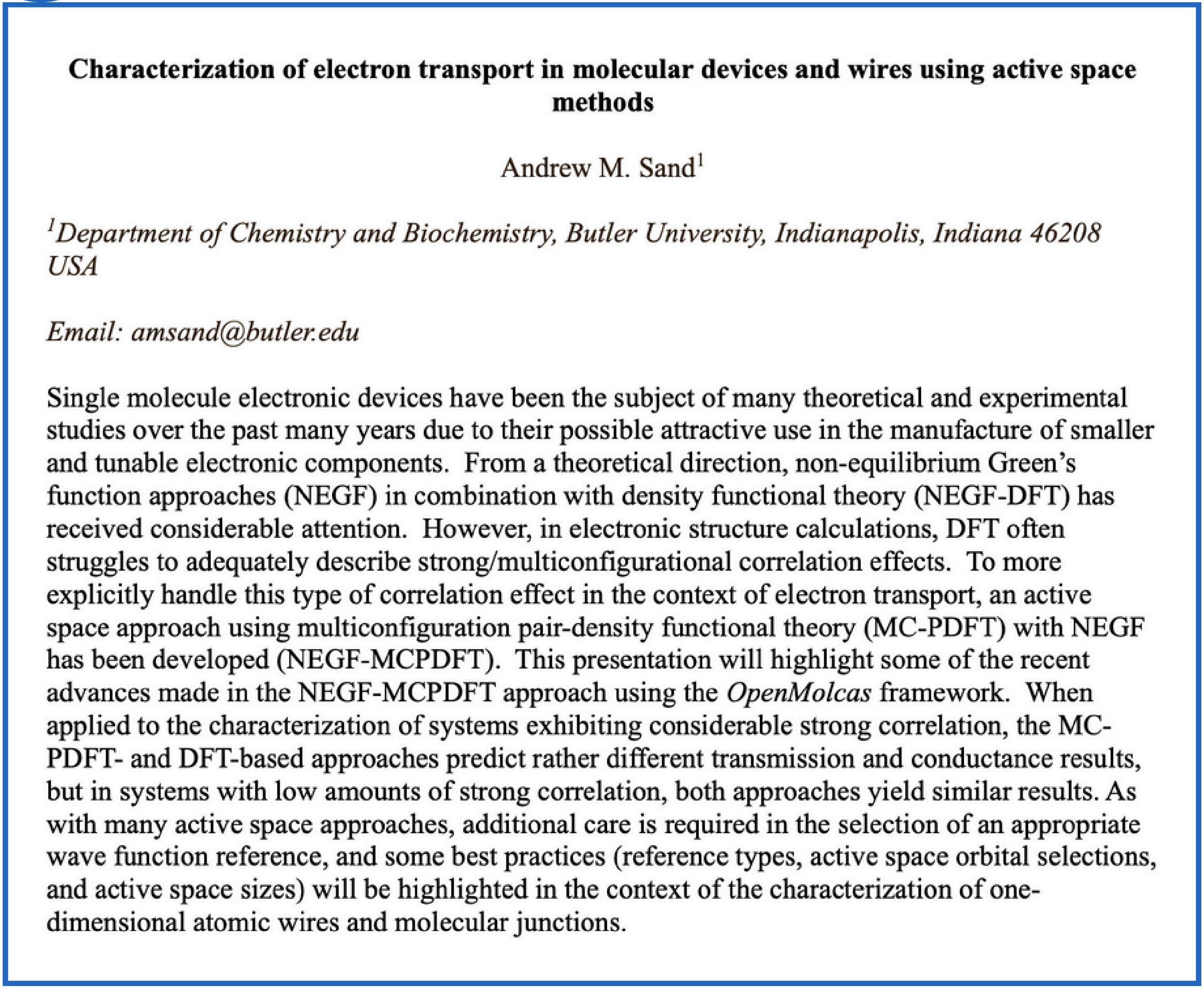
    b) QCES – Quantum Chemistry of Excited States (2024, 2025, Cluj) (https://www.molcas.org/QCES)
[2] a) Molecular Quantum Mechanics (master course at Lund University) (https://www.lunduniversity.lu.se/lubas/i-uoh-lu-KEMM58),
    b) Quantum chemistry at work (PhD course at Lund University) https://www.kilu.lu.se/en/education/doctoral-studies/doctoral-student-courses

Contr. talk



Characterization of electron transport in molecular devices and wires using active space methods

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Email: amsand@butler.edu

Single molecule electronic devices have been the subject of many theoretical and experimental studies over the past many years due to their possible attractive use in the manufacture of smaller and tunable electronic components. From a theoretical direction, non-equilibrium Green's function approaches (NEGF) in combination with density functional theory (NEGF-DFT) has received considerable attention. However, in electronic structure calculations, DFT often struggles to adequately describe strong/multiconfigurational correlation effects. To more explicitly handle this type of correlation effect in the context of electron transport, an active space approach using multiconfiguration pair-density functional theory (MC-PDFT) with NEGF has been developed (NEGF-MCPDFT). This presentation will highlight some of the recent advances made in the NEGF-MCPDFT approach using the *OpenMolcas* framework. When applied to the characterization of systems exhibiting considerable strong correlation, the MC-PDFT- and DFT-based approaches predict rather different transmission and conductance results, but in systems with low amounts of strong correlation, both approaches yield similar results. As with many active space approaches, additional care is required in the selection of an appropriate wave function reference, and some best practices (reference types, active space orbital selections, and active space sizes) will be highlighted in the context of the characterization of one-dimensional atomic wires and molecular junctions.

Invited talk

Interpolating wave functions to accelerate photochemical dynamics

George Booth, Yannic Rath, Kemal Atalar (King's College London)

Photochemical dynamics is an area where strong correlation and excited states (and their intersection) demand advances from computational methodologies, and are a strong motivation for further development. Coupled to that, we have to answer questions that take place on the long timescales of atomic (rather than electronic) motion. This is a huge challenge, because propagating atoms in time along with the explicit electronic structure entails a prohibitive number of electronic structure calculations at high accuracy. We will present our work to straddle this gap, with a simple yet surprisingly effective interpolation scheme, allowing for efficient inference of the correlated multi-state electronic wave function through chemical space, and coupling this to the explicit motion of the atoms undergoing reactive (photo-)chemistry. We will show that this also allows problems of discontinuities in electronic structure methods to be alleviated, and how this has enabled high-accuracy electronic structure to be coupled to real molecular dynamics with unprecedented accuracy, allowing for the first time molecules to move on the exact potential energy surface as provided by state-of-the-art correlated methods.

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Room-temperature quantum tunnelling at singularities drive enormous reaction speed-ups

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Singlet oxygen is an important reactive precursor in biochemistry, synthetic, atmospheric and environmental chemistry [1]. Its reactivity competes with the nonradiative decay to the triplet [2, 3], which is an intersystem crossing in the Marcus inverted regime. Calculating the decay rate constant with Fermi's Golden Rule (FGR) requires solutions to the nuclear Schrödinger equation, which is computationally infeasible for ab initio potential energy surfaces (PESs). Instanton theory [4, 5] is a semiclassical approximation to FGR that describes the reaction in terms of a tunnelling reaction mechanism and captures multidimensional tunnelling and zero-point energy effects. However, for this reaction, the correlation function contains a branch-point singularity and a new type of instanton is required to describe the tunnelling process. The branch-point instanton describes a completely new type of tunnelling at a singularity, where an infinite set of tunnelling paths contribute equally to the reaction mechanism [6]. Using branch-point instanton theory with multireference electronic-structure PESs, we find an enormous tunnelling speed-up of *27 orders of magnitude* compared to transition-state theory, with significant heavy-atom tunnelling, at *room temperature*. The instanton tunnelling mechanism correctly predicts the large experimentally-observed H_2O/D_2O kinetic isotope effect across a wide range of temperatures.

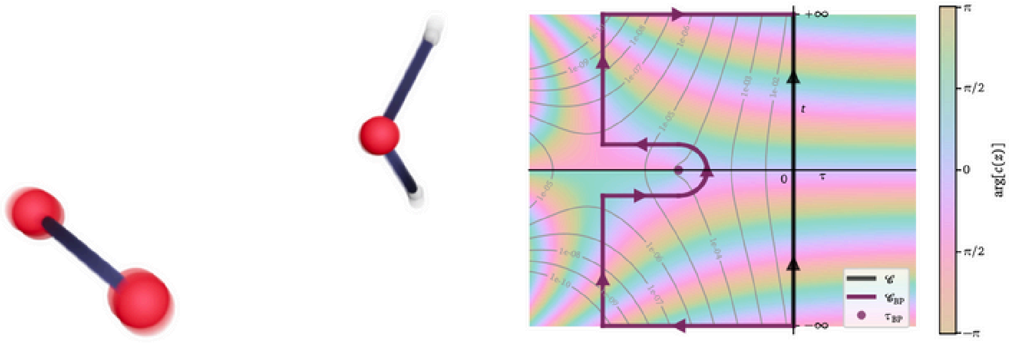

FIG. 1: (Left) The tunnelling mechanism of the $O_2 \cdots H_2O$ complex for the nonradiative decay to the triplet state. The motion of atoms involved in tunnelling is depicted with a motion blur effect. (Right) The complex domain plot of the correlation function with a singularity, together with the integration contours.

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Contr. talk

Ab Initio Multiple Spawning Nonadiabatic Dynamics with OpenMolcas

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In this talk, we want to introduce our very recent developments to propagate nonadiabatic dynamics with Ab Initio Multiple Spawning (AIMS) on potential energy surfaces calculated at CASPT2 level with OpenMolcas[1]. AIMS represents one of the highest standards of accuracy for nuclear propagation on coupled electronic states. It is derived from first principle and incorporates nonadiabatic and nuclear quantum effects by propagating, on different electronic states, coupled Gaussians that interact and exchange amplitude.

However, an accurate dynamics, requires accurate electronic structure properties. We interfaced PySpawn[2], an open-source implementation of the AIMS algorithm, with OpenMolcas to propagate the Gaussians on CASSCF and CASPT2 potential energy surfaces. As AIMS was previously only available in proprietary software, this implementation is unique, as it is the first fully open-source implementation of AIMS.

We extensively tested different CASPT2 flavors (MS,XMS,XDW and RMS) on the dynamics of fulvene, showing drastic differences between the relaxation with or without including PT2 correction and highlight imporant features of the different flavors, proposing a recommendation on the one to use for nonadiabatic dynamics.

Finally, we will show the latest update of the code, where a further interface with xTB was developed to model and capture solvent effects on nonadiabatic dynamics at the AIMS/CASPT2/GFN2-xTB level [3].

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Understanding the Excited States of an Iron(III) NHC Complex: Insights from Multiconfigurational Methods

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Photoactive iron(III) complexes bearing N-heterocyclic carbene ligands have recently emerged as promising candidates for sustainable photochemical applications, offering an Earth-abundant alternative to traditional ruthenium-based photosensitizers. Despite progress in ligand design, theoretical characterization of their low-lying excited states remains challenging due to the multiconfigurational nature of the d^5 open-shell ground state and the presence of near-degenerate metal-centered and charge-transfer states. In this work, we present a detailed multiconfigurational study of the electronically excited states of the cyclometallated Fe(III) complex $[Fe(ImP)_2]^+$. Using OpenMolcas, we used complete-active-space self-consistent field (CASSCF) and restricted-active-space self-consistent field (RASSCF) methods together with multireference perturbation theories and multiconfiguration pair-density functional theory (MC-PDFT) to investigate the manifold of excited doublet states. Special attention is given to active space selection, state-averaging schemes, solvation effects, and RAS partitioning strategies (Fig.1).

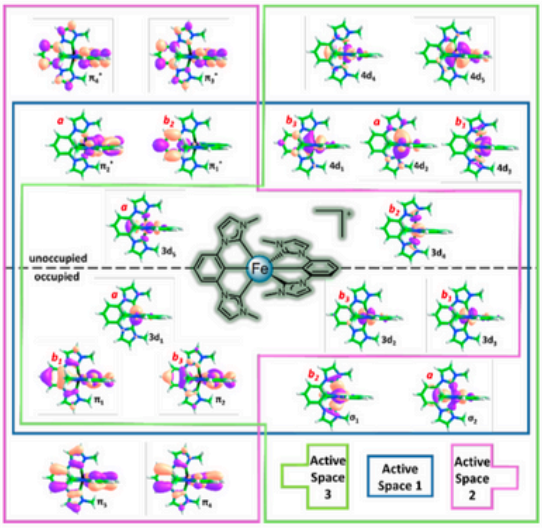

Fig.1. $[Fe(ImP)_2]^+$ compound and visual representation of the chosen active spaces and their orbital composition used in the multireference calculations.

Among the tested approaches, we identify a RASSCF strategy that offers results comparable to more demanding CASSCF while significantly reducing computational cost. In addition, we find that MC-PDFT provides a reliable and efficient alternative to traditional perturbation-based treatments. These findings demonstrate the value of tailored multiconfigurational approaches for modeling iron-based photoactive systems and offer practical guidance for future computational studies of complex transition metal photophysics.

Contr. talk

Characterizing Photoredox Active Transition Metal Catalysts with Extended Active-Space Wave Functions from Density Matrix Renormalization Group

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Controlled carbon–heteroatom bond formation via photoredox catalysis is crucial in organic synthesis, with nickel complexes offering a sustainable platform for light-driven transformations. Recent X-ray spectroscopic studies reveal pronounced multi-configurational (MC) behavior in catalytic Ni complexes, largely modulated by metal–ligand back-bonding[1] By employing state-of-the-art extended active spaces using density matrix renormalization group (DMRG) calculations, we aim to accurately identify and characterize the metal-to-ligand charge transfer (MLCT) excited states implicated in the catalytic reactivity. DMRG can address extended conjugation through large active spaces and improved reference wave functions.[2] Specifically, π-conjugated systems[3] and metal centers[4] are ideal applications for DMRG. Therefore we apply DMRG to incorporate the full ligand π-system and metal d-orbitals with second shell effects to accurately resolve the MLCT states in these metallaphotoredox catalysts. This study provides a foundation for future mixed quantum-classical dynamics simulations. We will integrate time-dependent density functional theory-based surface hopping simulations with transfer learning from DMRG-PDFT.[5] This framework has been effectively employed to obtain CASPT2 level dynamics simulations with a small number of energy calculations.[6] These simulations, to our knowledge, would represent the first application of DMRG-informed surface hopping to Ni-based systems, with implications for modeling photochemical reactivity in complex transition metal environments.

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A novel algorithm that couples Quantum Dynamics with Molecular Mechanics: study on the excitation energy transfer process of NADH solvated in water

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We present the development and implementation of a novel mixed QM/MM algorithm, designed to be applied for the simulation of excited state dynamics in solvent. While retaining the standard QM/MM partitioning features, the innovation lies in the treatment of both the nuclear and electronic degrees of freedom of the QM region at a fully quantum level of theory, hence the name QD/MM. This in turn allows for a to higher level of sophistication than commonly used methods, such as trajectory surface hopping.

To validate the algorithm, we applied it to analyze the Excitation Energy Transfer (EET) process of NADH solvated in water by tracking the populations of the three excited states involved in the relaxation pathway.

We compared the results obtained with those of a previous work [1], which studied the same EET process, in order to show that the solvent plays a critical role in determining the EET rate due to its effect on the energetics of the charge transfer state that mediates the population transfer.

The algorithm exploits the strengths of several quantum mechanical software packages, such as Quantics (for the QD part), AMBER (to compute all solvent-solvent terms), and OpenMolcas (required to compute QD-MM coupling terms). The implementation in the COBRAMM [2] suite facilitates the interface among the different software.

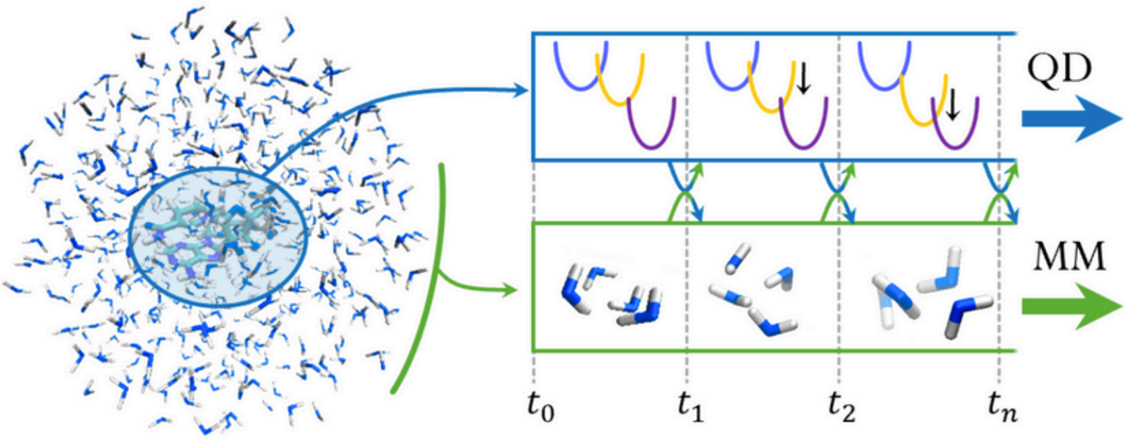

Figure 1: Schematic represantion of the QDMM algorithm workflow, applied on NADH solvated in water. At each time step (t) the QD and MM regions are interfaced with each other, allowing for frequent communication between the two levels of theory.

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Contr. talk

Ultrafast non-adiabatic dynamics via multiconfigurational Ehrenfest method

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The coupled dynamics of electrons and nuclei play an important role in understanding photophysics and photochemistry. While wave packet quantum dynamics are in principle exact, the computational cost is high for larger numbers of vibrational modes or involved electronic states. Thus, approximations to the exact dynamics have to be employed. The mean-field Ehrenfest dynamics represents a simple quantum-classical method where the nuclear dynamics is treated classically, driven by a force obtained from an average over several potential energy surfaces. The multiconfigurational Ehrenfest method uses precomputed mean-field Ehrenfest trajectories to construct a basis for a full quantum dynamics calculation, reproducing exact results in the completeness limit of infinitely many basis functions. For incomplete basis sets, the choice of starting points for the mean-field Ehrenfest trajectories influences the quality of the results. In the presented work, different ways of choosing these initial conditions are proposed and tested for small systems. In addition, the implementation strategy in the context of OpenMolcas will be discussed.

Time-resolved Spectroscopy with OpenMolcas: from quantum chemistry (through COBRAMM) to spectroscopy & insight

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OpenMolcas provides an ample range of high quality quantum chemistry data that constitute the foundation pillars for broad applications in chemistry and physics. In our group, we are interested in the simulation of time-resolved spectroscopic techniques. Over the years we have developed a variety of computational tools and interfaces to compute on-the-flight dynamics and simulate spectroscopy on top, designing a workflow to foster the production of spectra from quantum chemistry outputs. Most of these tools have been integrated in COBRAMM[1], our in-house program package with a combined quantum mechanical/molecular mechanical (QM/MM) framework to bridge the atomistic to the nano-scale and the electronic structure to the observables.

In this contribution, I will show a variety of spectroscopic techniques that can be readily obtained in COBRAMM on the specific case of 1,3-cyclohexadiene (CHD) photo-induced ring-opening dynamics. Among these, one accounts for: transient-absorption, time-resolved (TR) photoelectron spectroscopy (PES), TR X-ray absorption (XAS), TR XPES, ultrafast electron diffraction (UED). Notably, TRPES[2], TRXAS[3] and UED[4] of CHD have been experimentally recorded: a detailed comparison between our CASPT2 on-the-fly (fewest-switches surface hopping) dynamics and spectra with such experiments will be eventually performed, demonstrating the accuracy of our protocol for marrying quantum chemistry to state-of-the-art time-resolved spectroscopy simulation.

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Tunneling splitting in benzoic acid dimers from multi-level Jacobi field instanton theory

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Vibrational levels of molecules with symmetry-related minima exhibit a splitting pattern, the origin of which can be traced back to the tunneling motion. The magnitude of the splitting is directly related to the timescales of molecular rearrangements driven by the tunneling motion, offering a unique insight into the molecular dynamics.[1,2] Additionally, the sizes of the splittings are extremely sensitive to the potential energy barriers that separate different minima, making them indispensable experimental probes into the high-energy regions of potential energy surfaces. A reliable method for calculating the splitting would therefore provide a useful tool for estimating the accuracy of different electronic structure models in this regime.

Calculating the magnitudes of tunneling splitting using quantum mechanical methods is, however, a challenging task. Difficulties arise from the fact that these values can span multiple orders of magnitude, even within the same molecular system, necessitating highly converged quantum mechanical calculations, which can become numerically challenging even for small molecules. Furthermore, obtaining highly accurate values implies sampling a high-dimensional potential energy surface, as the use of reduced dimensionality models is known to have a significant impact on the results.

We present the semiclassical Jacobi field instanton theory[3–5] that does not suffer from the problems of quantum mechanical methods, while providing accurate values of tunneling splitting in full dimensionality. The only necessary ingredients for this approach are the optimized minimum action path and a modest number of sampled Hessians of the potential energy surface, making it an ideal candidate for the use with *ab initio* on-the-fly potential energies. We further extend this method with a multi-level approach to increase the computational efficiency by employing different electronic structure models for the path optimization, potential energy barrier calculation and Hessian evaluation. We apply this method to calculate the tunneling splittings of several benzoic acid dimers, which represents one of the largest calculation of tunneling splitting in full dimensionality to date.

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Contr.
talk

Recent Developments in Stochastic Complete Active Space Second-Order Perturbation Theory

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Multiconfigurational perturbation theory provides a systematically improvable way to correct active space wave functions for missing dynamic correlation. In this contribution, we present our implementation of FCIQMC-CASPT2 that enables the augmentation of active space wave functions optimised in the Full CI Quantum Monte Carlo framework [1] with Complete Active Space second-order Perturbation Theory [2] as implemented in OpenMolcas.

We show why stable results require strict fermionic positivity of the occurring reduced density matrices [3] and how we guarantee this property by means of histogramming in FCIQMC [4]. Compared to previous attempts at higher-order RDM sampling, the new approach is more robust and computationally cheaper, allowing us to apply it to chemically meaningful systems.

In multiple application examples on mono- and dinuclear transition metal clusters, including a Fe-porphyrinoid and a high-T_C nickelate superconductor, accuracy comparable to DMRG-CASPT2 with cumulant approximation [5] is demonstrated.

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Stochastic-SplitGAS: A Multi-Reference Perturbation Theory Based on the Stochastic Imaginary-Time Evolution of Effective Hamiltonians

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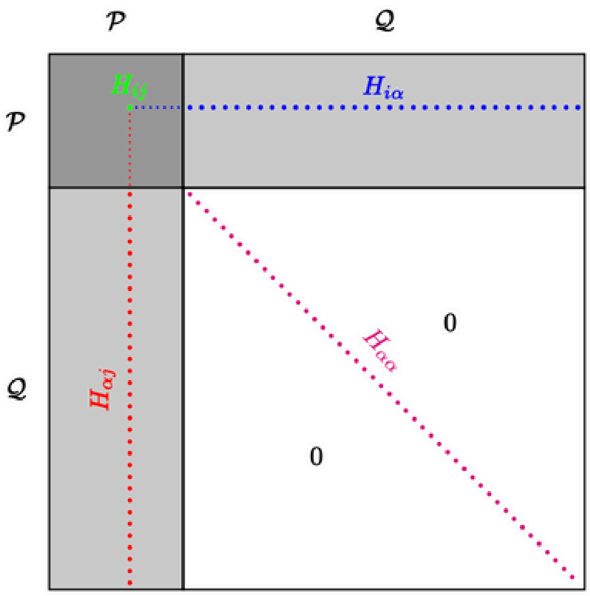
The study of complex electronic systems involving many unpaired electrons, such as polynuclear transition metal clusters at the centre of metalloproteins, is an important and challenging task in quantum chemistry. Accurate predictions of their electronic structures often require multireference methods, which are generally very expensive due to the exponential scaling of the electronic wave function with the number of correlated electrons and orbitals in the active space. Yet, dynamic correlation effects beyond the active space are to be accounted for. We present a stochastic variant of SplitGAS,[1,2] a perturbation theory strategy based on Löwdin's partitioning technique.[3] The configurational space is split into two parts, with the important configurations, forming the reference space, $\mathcal{P}$, and the more numerous configurations responsible for dynamic correlation effects forming the perturber space, $\mathcal{Q}$. Löwdin's working equations are utilised to form an effective Hamiltonian, which is explored stochastically. Test calculations were performed on Fe(II)-Porphyrin with a CAS(32,34) active space and 96 electrons in 153 orbitals in the perturber space.



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Poster

Free energy determinations with free energy perturbation theory and OpenMolcas

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Free-energy perturbation theory (FEPT) is a technique useful to determine the free energy change between two thermodynamic states in the electronic ground state. In this contribution, we shall see the adaptation to evaluate triplet energies (adiabatic singlet-triplet energy gaps) in macromolecular environments.[1] To illustrate it, we will see the performance of the adapted technique on the determination of the triplet energy of thymine in the isolated nucleotide in aqueous solution and in DNA. For that, FEPT molecular dynamics simulations were performed with the quantum chemistry / molecular mechanics (QM/MM) hybrid method. xTB, as implemented in QM3, was used for the dynamics and CASPT2, as implemented in OpenMolcas, was used to correct the free energies and obtain high-accurate estimations. The developed approach shall be useful for determining free energies of triplets and other states like ionic or charge separation states in any other macromolecular system with impact in biomedicine and materials science.

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Improving Photoabsorption Cross-Section Predictions for Atmospheric Compounds via Anharmonic Corrections in Nuclear Ensembles

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Accurate prediction of the light-induced behavior of atmospheric compounds is essential for understanding their photochemical lifetimes and reactivity in the troposphere. Many atmospheric compounds are transient or highly reactive, making experimental photoabsorption cross-section measurements challenging [1]. Computational approaches like the nuclear ensemble approach (NEA) [2] offer a practical alternative, allowing the prediction of electronic absorption spectra by averaging over vertical excitations sampled from a ground-state nuclear distribution. However, NEA implementations commonly rely on Wigner distributions constructed under the harmonic approximation, which can inadequately represent low-frequency anharmonic modes in flexible molecules [3,4].

In this work, we propose the incorporation of anharmonic corrections into the Wigner distribution employed for generating nuclear ensembles using the Newton-X software [5]. This improved sampling approach is subsequently applied to the calculation of electronic absorption spectra using multireference quantum chemical methods (RASSCF/CASPT2) within the OpenMolcas framework. The protocol is integrated with MULTISPEC, a tool developed in our group for constructing photochemical observables and convoluted spectra from ensemble-based data. The ultimate goal is to produce more realistic absorption cross-sections in the visible range, thereby enabling more accurate predictions of photolysis rates and light-induced reactivity in the troposphere. This contribution presents the early stages of a methodology under development and underscores its potential to improve the representation of compounds in atmospheric chemical models.

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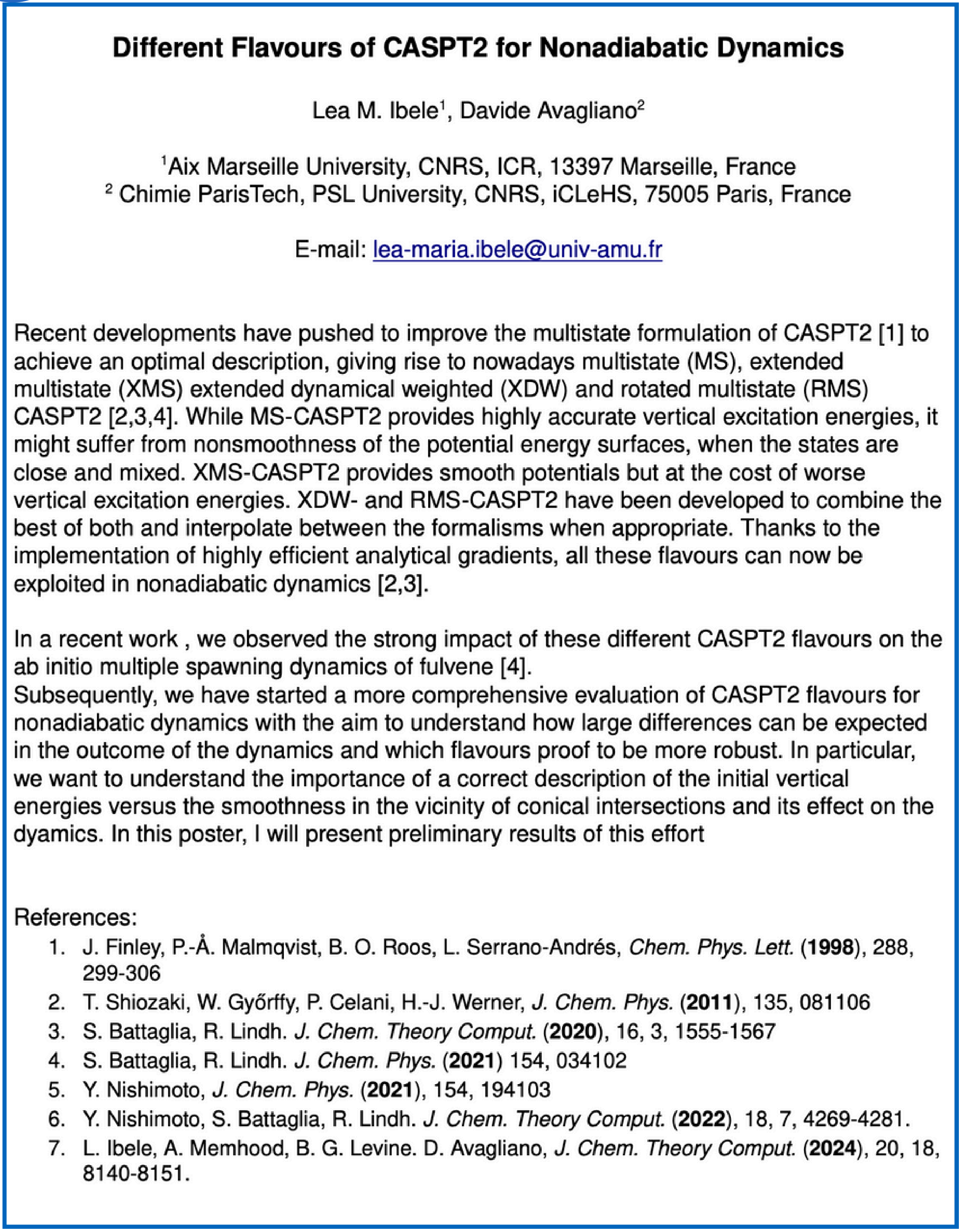

Different Flavours of CASPT2 for Nonadiabatic Dynamics

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Recent developments have pushed to improve the multistate formulation of CASPT2 [1] to achieve an optimal description, giving rise to nowadays multistate (MS), extended multistate (XMS) extended dynamical weighted (XDW) and rotated multistate (RMS) CASPT2 [2,3,4]. While MS-CASPT2 provides highly accurate vertical excitation energies, it might suffer from nonsmoothness of the potential energy surfaces, when the states are close and mixed. XMS-CASPT2 provides smooth potentials but at the cost of worse vertical excitation energies. XDW- and RMS-CASPT2 have been developed to combine the best of both and interpolate between the formalisms when appropriate. Thanks to the implementation of highly efficient analytical gradients, all these flavours can now be exploited in nonadiabatic dynamics [2,3].

In a recent work , we observed the strong impact of these different CASPT2 flavours on the ab initio multiple spawning dynamics of fulvene [4].
Subsequently, we have started a more comprehensive evaluation of CASPT2 flavours for nonadiabatic dynamics with the aim to understand how large differences can be expected in the outcome of the dynamics and which flavours proof to be more robust. In particular, we want to understand the importance of a correct description of the initial vertical energies versus the smoothness in the vicinity of conical intersections and its effect on the dyamics. In this poster, I will present preliminary results of this effort

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Refining Initial Condition Preparation for Surface Hopping by Including Explicit Laser Pulses

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The rapid development of femtochemistry over the past decades has revolutionized our understanding of ultrafast photochemical and photophysical phenomena. Nowadays, a plethora of ultrafast spectroscopic techniques allow for the direct observation of molecular dynamics on few-femtosecond timescales. The interpretation of such experiments is greatly facilitated by nonadiabatic molecular dynamics simulations which provide key insights into excited-state lifetimes, energy transfer mechanisms, and reaction pathways. Significant progress has been made in the development of electronic structure methods and nonadiabatic methods. However, the treatment of photoexcitation, the origin of the dynamics processes, often remains an oversimplified aspect in most surface hopping (SH) simulations[1], typically implemented as a delta-pulse excitation with energy-window-based initial state selection. These simplifications are owed to the high computational cost of explicit laser pulse incorporation, but neglect the true spatiotemporal and energetic characteristics of laser pulses. In this contribution, we introduce an alternative excitation strategy within the SHARC package[2] using explicit laser pulses. We take an ensemble of randomly sampled initial conditions and apply a laser pulse to a set of computationally inexpensive frozen-nuclei trajectories. Using the global flux SH formalism[3] and stochastic excited-state selection, we determine the initially excited electronic state and the excitation time from the trajectory results. Based on the so-selected initial states, the actual SH trajectories[2] are subsequently launched. The excitation time is applied in a post-processing step by shifting all trajectories accordingly. Our method captures diverse laser pulse characteristics—such as bandwidth, temporal spread, and polarization. It also enables the treatment of chirped and non-plane-wave pulses, such as tightly focused beams that do not exhibit the typical relationship between electric and magnetic fields[4]. We validate the method against simulations that include nuclear motion and discuss its applicability in complex photochemical scenarios.

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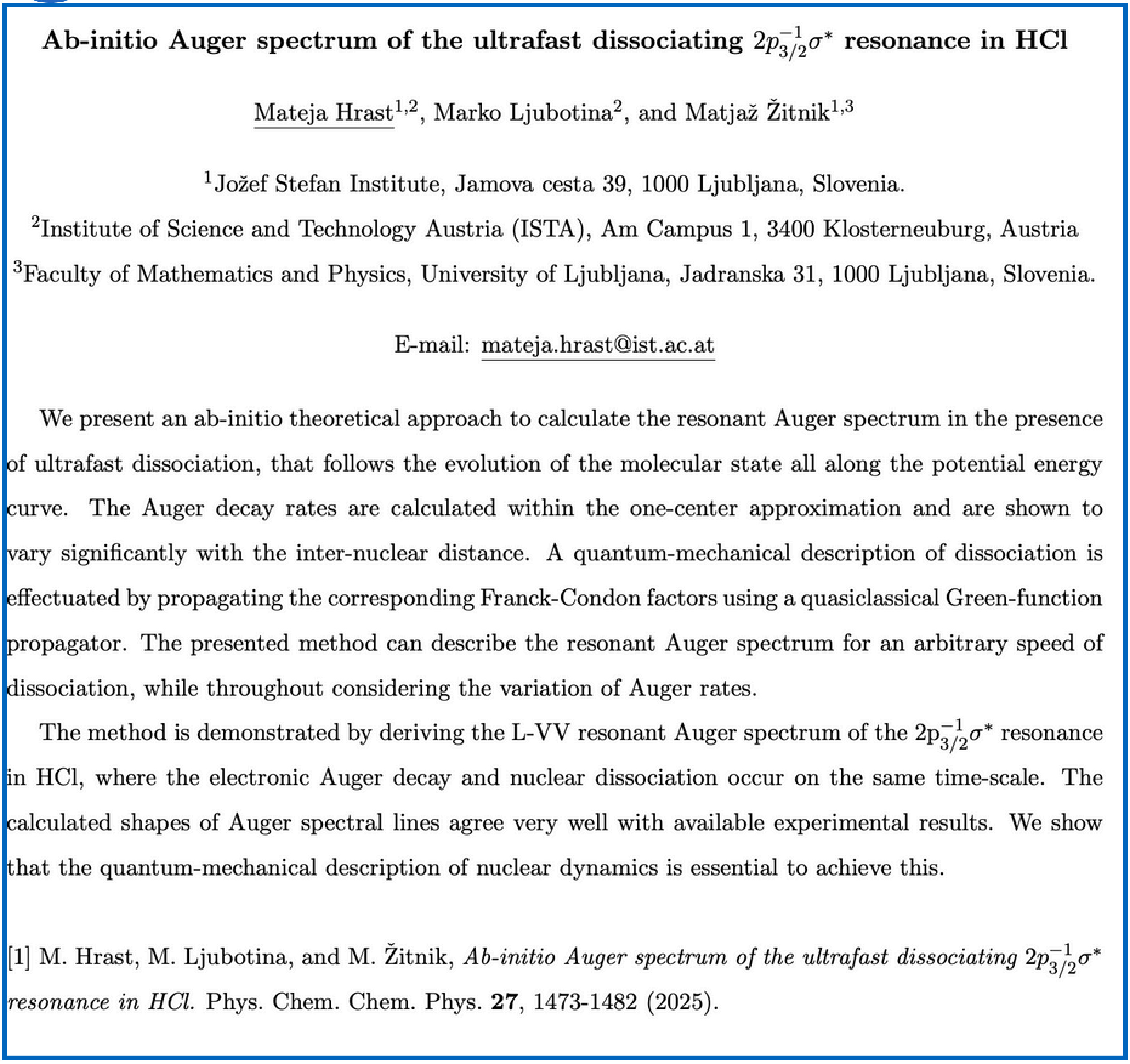
Poster



Ab-initio Auger spectrum of the ultrafast dissociating $2p_{3/2}^{-1}\sigma^*$ resonance in HCl

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We present an ab-initio theoretical approach to calculate the resonant Auger spectrum in the presence of ultrafast dissociation, that follows the evolution of the molecular state all along the potential energy curve. The Auger decay rates are calculated within the one-center approximation and are shown to vary significantly with the inter-nuclear distance. A quantum-mechanical description of dissociation is effectuated by propagating the corresponding Franck-Condon factors using a quasiclassical Green-function propagator. The presented method can describe the resonant Auger spectrum for an arbitrary speed of dissociation, while throughout considering the variation of Auger rates.

The method is demonstrated by deriving the L-VV resonant Auger spectrum of the $2p_{3/2}^{-1}\sigma^*$ resonance in HCl, where the electronic Auger decay and nuclear dissociation occur on the same time-scale. The calculated shapes of Auger spectral lines agree very well with available experimental results. We show that the quantum-mechanical description of nuclear dynamics is essential to achieve this.

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Dyson-density approach to charge-transfer excitons

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Understanding molecular aggregates and exciton dynamics is crucial to designing functional materials and molecular devices, and theoretical calculations offer indispensable help in it. In this context, not only excitons due to local excitations but also processes accompanied by a charge transfer from one monomer to the other can play an important role. The presented work extends a previously implemented protocol for Frenkel excitons [1], which used locally excited multiconfigurational wave functions, to include a single-particle charge transfer effect. To formulate the matrix elements of the aggregate Hamiltonian in the basis of multiconfigurational wave functions, attachment/detachment Dyson orbitals and Dyson densities for the monomers were employed, where the coupling terms appear in different orders of intermolecular overlap. The computational protocol is implemented in OpenMolcas as extension of the previously implemented protocol for Frenkel excitons [1] and tested on typical charge-transfer pairs.

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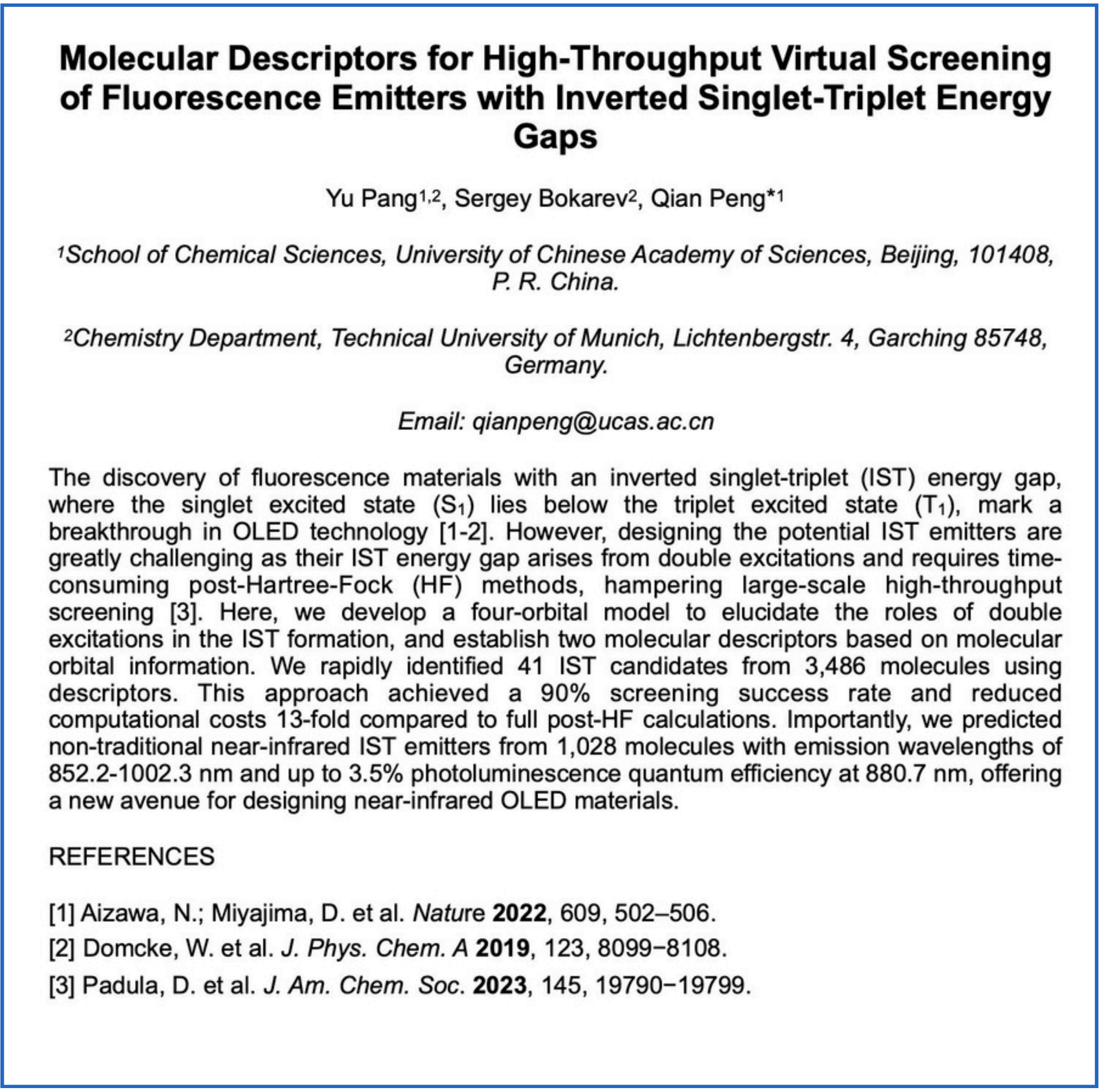
Poster



Molecular Descriptors for High-Throughput Virtual Screening of Fluorescence Emitters with Inverted Singlet-Triplet Energy Gaps

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The discovery of fluorescence materials with an inverted singlet-triplet (IST) energy gap, where the singlet excited state (S_1) lies below the triplet excited state (T_1), mark a breakthrough in OLED technology [1-2]. However, designing the potential IST emitters are greatly challenging as their IST energy gap arises from double excitations and requires time-consuming post-Hartree-Fock (HF) methods, hampering large-scale high-throughput screening [3]. Here, we develop a four-orbital model to elucidate the roles of double excitations in the IST formation, and establish two molecular descriptors based on molecular orbital information. We rapidly identified 41 IST candidates from 3,486 molecules using descriptors. This approach achieved a 90% screening success rate and reduced computational costs 13-fold compared to full post-HF calculations. Importantly, we predicted non-traditional near-infrared IST emitters from 1,028 molecules with emission wavelengths of 852.2-1002.3 nm and up to 3.5% photoluminescence quantum efficiency at 880.7 nm, offering a new avenue for designing near-infrared OLED materials.

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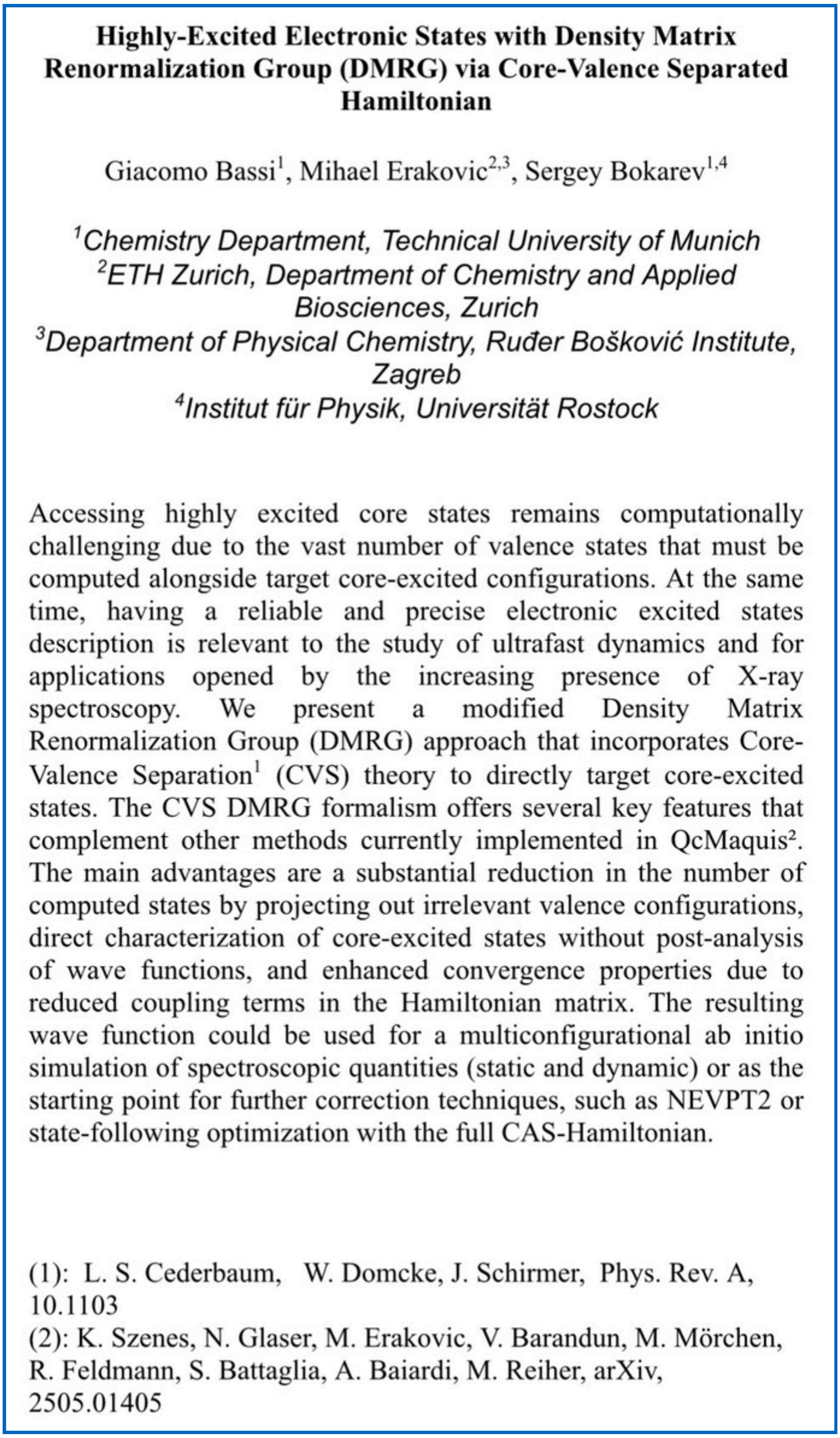
Poster



Highly-Excited Electronic States with Density Matrix Renormalization Group (DMRG) via Core-Valence Separated Hamiltonian

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Accessing highly excited core states remains computationally challenging due to the vast number of valence states that must be computed alongside target core-excited configurations. At the same time, having a reliable and precise electronic excited states description is relevant to the study of ultrafast dynamics and for applications opened by the increasing presence of X-ray spectroscopy. We present a modified Density Matrix Renormalization Group (DMRG) approach that incorporates Core-Valence Separation[1] (CVS) theory to directly target core-excited states. The CVS DMRG formalism offers several key features that complement other methods currently implemented in QcMaquis[2]. The main advantages are a substantial reduction in the number of computed states by projecting out irrelevant valence configurations, direct characterization of core-excited states without post-analysis of wave functions, and enhanced convergence properties due to reduced coupling terms in the Hamiltonian matrix. The resulting wave function could be used for a multiconfigurational ab initio simulation of spectroscopic quantities (static and dynamic) or as the starting point for further correction techniques, such as NEVPT2 or state-following optimization with the full CAS-Hamiltonian.

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