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2025 CESTC

BOOK OF ABSTRACTS

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Conference History

Welcome to the **20th Central European Symposium on Theoretical Chemistry**! This edition marks a special milestone for our community. Over the years, CESTC has grown into more than just a conference – it's become a place to share ideas, start collaborations, and build a strong network of researchers and friendships that have lasted well beyond the meetings. We look forward to continuing this tradition for many years to come.

The following list reflects the rich history of the symposium and the places that have hosted this series over the years:

- 2025 Stará Lesná, Slovakia
- 2024 Sveti Martin na Muri, Croatia
- 2022 Balatonszárszó, Hungary
- 2019 Burg Schlaining, Austria
- 2018 Srní, Czech Republic
- 2017 Wisla, Poland
- 2015 Banská Bystrica, Slovakia
- 2014 Nagybörzsöny, Hungary
- 2013 Znojmo, Czech Repbublic
- 2012 Mariapfarr, Austria
- 2011 Toruń, Poland
- 2010 Nový Smokovec, Slovakia
- 2009 Dobogókő, Hungary
- 2008 Hejnice, Czech Republic
- 2007 Litschau, Austria
- 2006 Zakopane, Poland
- 2005 Šachtičky, Slovakia
- 2004 Tihany, Hungary
- 2003 Nové Hrady, Czech Republic
- 2002 Zwettl, Austria

	MONDAY	TUESDAY	WEDNESDAY	THURSDAY
09:00		**Session 3 (Jiří Pittner)**	**Trips / Hikes**	**Session 9 (Miroslav Medveď)**
		IL4 Bím		IL12 Tandarić
09:40		C6 Piteša		C21 Fedorov
10:00		C7 Bende		C22 Sládek
10:20		C8 Grabarz		C23 Poliak
10:40		Coffee break		Coffee break
11:00	**Registration**	**Session 4 (Monika A. Musiał)**		**Session 10 (Pavel Neogrády)**
		IL5 Sangiogo-Gil		C24 Lechner
11:20				C25 Vénosová
11:40		C9 Zams		C26 Niedzielski
12:00		C10 Sheik		**Closing Ceremony**
12:20		Lunch	Lunch	Lunch
14:00	**Session 1 (Jozef Noga)**	**Session 5 (Péter G. Szalay)**	**Session 7 (Ágnes Szabados)**	
	IL1 Grabowski	IL6 Maurer	IL9 Konečný	
14:40	C1 Derzsi	C11 Benková	C16 Dutta	
15:00	C2 Podrojková	C12 Fárníková	C17 Musiał	
15:20	C3 Tokár	C13 Onija-Ioan	C18 Morita	
15:40	Coffee break	Coffee break	Coffee break	
16:00	**Session 2 (Péter Surján)**	**Session 6 (Miroslav Urban)**	**Session 8 (Michał Przybytek)**	
	IL2 Lazar	IL7 Rosta	IL10 Tomza	
16:40	IL3 Gešvandtnerová	IL8 Kállay	IL11 Cvitaš	
17:20	C4 Śmiga	C14 Kedžuch	C19 Tecmer	
17:40	C5 Straka	C15 Šimunek	C20 Ćosićová	
18:00	Dinner	Dinner		
19:00			**Banquet**	
20:00	**Poster Session A**	**Poster Session B**		
22:00				

Monday		**8th Sept.**
11:00		**Registration**
Chairperson	Jozef Noga	
14:00	Ireneusz Grabowski	An Evaluation of the Hybrid KS DFT Functionals Based on the KS Exchange-Correlation Potentials
14:40	Mariana Derzsi	Metal-metal interactions in an open d-shell system with cuprite structure
15:00	Natália Podrojková	Theoretical Exploration of HER Mechanisms on Transition Metal Phosphide Surfaces
15:20	Kamil Tokár	DFT Insights into Defect and Temperature-Dependent Band Gaps in Halide Perovskites
15:40		**Coffee break**
Chairperson	Péter Surján	
16:00	Petr Lazar	Going beyond standard DFT in periodic systems: the story of fluorographene
16:40	Monika Gešvandtnerová	Isobutanol conversion catalyzed by acidic zeolites
17:20	Szymon Śmiga	Simplified, Physically Motivated, and Broadly Applicable Range-Separation Tuning
18:40	Michal Straka	Actinide-actinide bonding in fullerenes. A challenge for theory
18:00		**Dinner**
20:00		**Poster Session A**
22:00		**End of the Official Programme**

Tuesday		**9th Sept.**
Chairperson	Jiří Pittner	
09:00	Daniel Bím	Electronic Structure Insights into Reactivity Across Ground and Excited States in Nickel Photocatalysts
09:40	Tomislav Piteša	Electronic Transitions in Supramolecular Aggregates
10:00	Attila Bende	Intermolecular-type conical intersections in molecular dimers
10:20	Anna M. Grabarz	Towards accurate simulations of the optical signatures of fluorophores
10:40		**Coffee break**
Chairperson	Monika A. Musiał	
11:00	Eduarda Sangiogo Gil	Methods for simulating excited-state dynamics in complex systems and environments
11:40	Joanna Zams	Cu(I)-based heteroleptic photosensitizers – a theoretical analysis of the low-lying excited states
12:00	Haseena Sheik	Study of Photorelaxation Pathways in ^{7}H and ^{9}H tautomers of 2,6-Diaminopurine
12:20		**Lunch**
Chairperson	Péter G. Szalay	
14:00	Reinhard Maurer	Machine Learning Surrogate Models of Electronic Structure for Quantum Dynamics and Inverse Design
14:40	Zuzana Benková	Comparison of interactions of proteins with poly(ethylene oxide) layers in two setups
15:00	Karolína Fárníková	Modeling the uptake of small oxidized organic molecules by gas-phase hydrated nitric acid clusters
15:20	Radu O. Ioan	Super-reduced metals in enzymes: why and how? The case of cobalamin and coenzyme F_{430}
15:40		**Coffee break**

Chairperson	Miroslav Urban	
16:00	Edina Rosta	Nature counts to three: Universal Mg-pinch motif polarizes the cleaved bond in NTP-processing enzymes
16:40	Mihály Kállay	Basis-set limit MP2 correlation energies for large molecules
17:20	Stanislav Kedžuch	Single-reference coupled cluster theory for systems with strong correlation extended to excited states
17:40	Ján Šimunek	Accelerated Hartree-Fock approach via reduced virtual orbital space
18:00		**Dinner**
20:00		**Poster Session B**
22:00		**End of the Official Programme**

Wednesday		**10th Sept.**
09:00		**Trips/Hikes**
12:20		**Lunch**
Chairperson	Ágnes Szabados	
14:00	Lukáš Konečný	From relativistic spectroscopy to quantum electrodynamics and back
14:40	Achintya K. Dutta	Low-cost Relativistic Coupled Cluster Method Based on Frozen Natural Spinors
15:00	Monika A. Musiał	Multereference coupled cluster method for the description of the dissociation of a single bond: the easy way
15:20	Masato Morita	Ab initio calculation of magnetic Feshbach resonances in ultracold collisions between Rb (^2S) and AlF($^1\Sigma^+$)
15:40		**Coffee break**
Chairperson	Michał Przybytek	
16:00	Michał Tomza	Ultracold highly magnetic and polar molecules for quantum simulation and new physics search
16:40	Marko T. Cvitaš	Tunneling splittings in vibrational spectra of molecules using modified WKB in Cartesian coordinates
17:20	Paweł Tecmer	pCCD-based computational strategies for large-scale modeling of organic electronics in the PyBEST software package
17:40	Martina Ćosićová	Neural network based algorithms for diabatization of electronic bases
19:00		**Banquet**
22:00		**End of the Official Programme**

Thursday		**11th Sept.**
Chairperson	Miroslav Medveď	
09:00	Tana Tandarić	Application of Free Energy Perturbation in Structure-Based Drug Design: Insights from Adenosine Receptors
09:40	Dmitri G. Fedorov	Quantum-mechanical calculations of large molecular systems and analyses of interactions
10:00	Vladimír Sládek	Identifying residue relevance in biomolecular interfaces – beyond reading the tea leaves
10:20	Peter Poliak	Advancing the Buffer Region Neural Network Embedding Scheme (BuRNN) for Complex Molecular Environments
10:40		**Coffee Break**
Chairperson	Pavel Neogrády	
11:00	Patrick Lechner	Spin Frustration in Triangular Fe(III) MOFs: A Hidden Key to Reactivity
11:20	Barbora Vénosová	Small dots, Big effects: How size and functional groups affect the electronic and optical properties of MXene Quantum Dots
11:40	Grzegorz M. Niedzielski	A density-based energy decomposition scheme for interacting fragments in periodic models and its insights into bonding and descriptors
12:00		**Closing Ceremony**

List of Invited Lectures

Bím, D. (IL4, Tuesday 09:00): *Electronic Structure Insights into Reactivity Across Ground and Excited States in Nickel Photocatalysts*

Cvitaš, M. (IL11, Wednesday 16:40): *Tunneling splittings in vibrational spectra of molecules using modified WKB in Cartesian coordinates*

Gešvandtnerová, M. (IL3, Monday 16:40): *Isobutanol conversion catalyzed by acidic zeolites*

Sangiogo Gil, E. (IL5, Tuesday 11:00): *Methods for simulating excited-state dynamics in complex systems and environments*

Grabowski, I. (IL1, Monday 14:00): *An Evaluation of the Hybrid KS DFT Functionals Based on the KS Exchange-Correlation Potentials*

Kállay, M. (IL8, Tuesday 16:40): *Basis-set limit MP2 correlation energies for large molecules*

Konečný, L. (IL9, Wednesday 14:00): *From relativistic spectroscopy to quantum electrodynamics and back*

Lazar, P. (IL2, Monday 16:00): *Going beyond standard DFT in periodic systems: the story of fluorographene*

Maurer, R. (IL6, Tuesday 14:00): *Machine Learning Surrogate Models of Electronic Structure for Quantum Dynamics and Inverse Design*

Rosta, E. (IL7, Tuesday 16:00): *Nature counts to three: Universal Mg-pinch motif polarizes the cleaved bond in NTP-processing enzymes*

Tandarić, T. (IL12, Thursday 09:00): *Application of Free Energy Perturbation in Structure-Based Drug Design: Insights from Adenosine Receptors*

Tomza, M. (IL10, Wednesday 16:00): *Ultracold highly magnetic and polar molecules for quantum simulation and new physics search*

List of Contributed Talks

Bende, A. (IC7, Tuesday 10:00): *Intermolecular-type conical intersections in molecular dimers*

Benková, Z. (IC11, Tuesday 14:40): *Comparison of interactions of proteins with poly(ethylene oxide) layers in two setups*

Ćosićová, M. (IC20, Wednesday 17:40): *Neural network based algorithms for diabatization of electronic bases*

Derzsi, M. (IC1, Monday 14:40): *Metal-metal interactions in an open d-shell system with cuprite structure*

Dutta, A. (IC16, Wednesday 14:40): *Low-cost Relativistic Coupled Cluster Method Based on Frozen Natural Spinors*

Fárníková, K. (IC12, Tuesday 15:00): *Modeling the uptake of small oxidized organic molecules by gas-phase hydrated nitric acid clusters*

Fedorov, D. (IC21, Thursday 09:40): *Quantum-mechanical calculations of large molecular systems and analyses of interactions*

Grabarz, A. (IC8, Tuesday 10:20): *Towards accurate simulations of the optical signatures of fluorophores*

Ioan, R. (IC13, Tuesday 15:20): *Super-reduced metals in enzymes: why and how? The case of cobalamin and coenzyme* F_{430}

Kedžuch, S. (IC14, Tuesday 17:20): *Single-reference coupled cluster theory for systems with strong correlation extended to excited states*

Lechner, P. (IC24, Thursday 11:00): *Spin Frustration in Triangular Fe(III) MOFs: A Hidden Key to Reactivity*

Morita, M. (IC18, Wednesday 15:20): *Ab initio calculation of magnetic Feshbach resonances in ultracold collisions between Rb* (^2S) *and AlF*($^1\Sigma^+$)

Musiał, M. (IC17, Wednesday 15:00): *Multereference coupled cluster method for the description of the dissociation of a single bond: the easy way*

Niedzielski, G. (IC26, Thursday 11:40): *A density-based energy decomposition scheme for interacting fragments in periodic models and its insights into bonding and descriptors*

Piteša, T. (IC6, Tuesday 09:40): *Electronic Transitions in Supramolecular Aggregates*

Podrojková, N. (IC2, Monday 15:00): *Theoretical Exploration of HER Mechanisms on Transition Metal Phosphide Surfaces*

Poliak, P. (IC23, Thursday 10:20): *Advancing the Buffer Region Neural Network Embedding Scheme (BuRNN) for Complex Molecular Environments*

Sheik, H. (IC10, Tuesday 12:00): *Study of Photorelaxation Pathways in ^{7}H and ^{9}H tautomers of 2,6-Diaminopurine*

Šimunek, J. (IC15, Tuesday 17:40): *Accelerated Hartree-Fock approach via reduced virtual orbital space*

Sládek, V. (IC22, Thursday 10:00): *Identifying residue relevance in biomolecular interfaces – beyond reading the tea leaves*

Straka, M. (IC5, Monday 18:40): *Actinide-actinide bonding in fullerenes. A challenge for theory*

Śmiga, S. (IC4, Monday 17:20): *Simplified, Physically Motivated, and Broadly Applicable Range-Separation Tuning*

Tecmer, P. (IC19, Wednesday 17:20): *pCCD-based computational strategies for large-scale modeling of organic electronics in the PyBEST software package*

Tokár, K. (IC3, Monday 15:20): *DFT Insights into Defect and Temperature-Dependent Band Gaps in Halide Perovskites*

Vénosová, B. (IC25, Thursday 11:20): *Small dots, Big effects: How size and functional groups affect the electronic and optical properties of MXene Quantum Dots*

Zams, J. (IC9, Tuesday 11:40): *Cu(I)-based heteroleptic photosensitizers – a theoretical analysis of the low-lying excited states*

List of Posters

(Posters marked by an asterisk are part of the poster competition presented by PhD students)

PA1 **Alharzali, N.**: *Hydroxyl radical initiated oxidation of methylmercury hydroxide in the aqueous phase: A theoretical study*

PA2* **Andreides, B.**: *Progress in Generating Accurate Atomic and Molecular Gaussian Rydberg Basis Sets*

PA3 **Andrzejak, M.**: *Reorganization energies of extended organic oligomers from DFT perspective*

PA4* **Barcza, B.**: *A Generalized Framework for Excited-State Coupling in Molecular Fragments based on Second Quantization*

PA5* **Behjou, S.**: *Tailored EOM-CC Methods for Electron Attachment Energies*

PA6* **Boršová, V.**: *Molecular Dynamics Investigation of Flavonoid–HSA Interactions*

PA7 **Bucinsky, L.**: *Transition metal complexes: closed shell state stability and DFT vs. CASSCF comparison*

PA8 **Budzák, Š.**: *Global Optimization of Cluster Structures via Genetic Algorithm*

PA9 **Bujdák, R.**: *A Computational Study of NiO Polymorphism*

PA10* **Chakraborty, R.**: *Molecular Properties with pCCD-based Methods*

PA11* **Chirchir, G.**: *Integral Package for More Flexible Quantum Chemical Simulations*

PA12* **Cosma, S.**: *No Heme-Chlorite Adduct in the Catalytic Cycle of Chlorite Dismutase: Insights From QM/MM and Dynamics Calculations*

PA13 **Dawson, W.**: *Reducing Numerical Precision Requirements in Quantum Chemistry Calculations*

PA14 **Demel, O.**: *Tailored coupled cluster study of singlet-triplet gaps in cyclazine, heptazine, and cycloborane*

PA15* **Dihingia, H.**: *Exploring Intermolecular Interaction Through Variational Lens*

PA16 **Dubecký, M.**: *From Fermion Sign Structure to Static Correlation*

PA17* **Dunárová, A.**: *Comprehensive Docking Prediction of Compounds Targeting the SARS-CoV-2 Main Protease*

PA18* **Elmaadawy, M.**: *Non-Bonded Interactions in Empirical Force Fields: Revisiting Parametrization in Classical Models*

PA19 **Erakovic, M.**: *Spin-free SC-NEVPT2 Method for the Quantum Embedding of the Open-Shell Systems*

PA20* **Fabušová, D.**: *Theoretical prediction of novel palladium oxide phases based on ion beam synthesis experimental data*

PA21 **Filgas, J.**: *UV Chromophore Excited with Visible Light: CO Release from Flavonol*

PA22* **Melo Flores, B.**: *Relativistic iterative linear damped response TDDFT solver for predicting X-ray absorption spectra of open-shell molecules*

PA23* **Fraško, P.**: *In silico modeling of reactions using machine-learned neural networks*

PA24 **Gall, M.**: *Improving docking score predictions through training dataset enrichment*

PA25 **Gałyńska, M.**: *Investigating Excited-State Charge Transfer in Donor–Bridge–Acceptor Systems with EOM-PCCD+S*

PA26* **Gombás, A.**: *The effect of orbital optimization and correlation correction in spin-unrestricted geminal models*

PA27* **Hlinčík, A.**: *DFT and CASSCF Cr^I–Cr^I bond characterization and what can do quantum crystallography*

PA28* **Hurajt, A.**: *Accurate nuclear magnetic dipole moments of ^{77}Se and $^{123,125}Te$ isotopes*

PA29* **Jahani, S.**: *Efficient Koopmans'-Based Orbital Energy Predictions for Organic Solar Cells Using pCCD type methods.*

PA30 **Jelemenska, I.**: *The catalytic effect of copper complexes with non- innocent pentan-2,4-dione bis(amidrazones) ligand in CuAAC reaction. DFT study.*

PA31* **Kolářová, E.**: *Non-canonical α/γ backbone conformations in DNA and protein-DNA complexes*

PA32 **Komorovsky, S.**: *Relativistic DFT methods for predicting EPR parameters of species containing heavy elements*

PA33* **Kopczyński, M.**: *Dressed pCCD: Efficient Modeling of Electron Correlation*

PA34* **Kováčová, A.**: *On the keto-enol tautomerism of polycyclic aromatic hydrocarbons*

PB1 **Kóňa, J.**: *Theoretical study on structure and interactions between cytomegalovirus glycoprotein UL141 and small glycomimetic antagonists*

PB2* **Lakmuang, C.**: *Mechanistic Study of the Conversion of Primary Alcohols and Butadiene to Branched Ketone Using Rhodium Catalyst*

PB3 **Lemken, F.**: *Through-Space Spin-Spin Coupling Pathway Propagated via π-Orbitals*

PB4* **Lévárdi, Á.**: *ML-based prediction of protein-ligand binding affinities utilizing atomic representations*

PB5* **Maková, M.**: *Voxel-based Computational Quantification of Rodent Brain MRI data*

PB6 **Malcek, M.**: *Transition metal clustering on carbon-based nanostructures and their hydrogen storage properties*

PB7* **Martinka, J.**: *A Descriptor Is All You Need: Accurate Machine Learning of Nonadiabatic Coupling Vectors*

PB8* **Martinović, M.**: *Stability indicators of hydrogenated Fullerenes*

PB9 **Matúška, J.**: *Targeted enrichment of the training dataset as a path to more accurate predictions*

PB10 **Medveď, M.**: *Computational Insights into Photochromism of Triarylhydrazones*

PB11 **Mester, D.**: *Density-based basis-set correction within local approximations*

PB12 **Mihálka, É.**: *Explicitly correlated geminal-based perturbation*

PB13* **Müllerová, S.**: *A Computational Study of Hydrogen Adsorption on Nickel-Modified Borophene*

PB14 **Munzarová, M.**: *Exploring the Regioselectivity of Diels-Alder reactions of new 2,6-disubstituted benzoquinones by means of quantum chemistry*

PB15* **Myšák, D.**: *Computational Modelling of Glutamate Dehydrogenase in Crowded Environment with Focus on the Active Site*

PB16 **Novotny, J.**: *Identification of distinct spin transmission pathways in acac ligand coordinated to Ru(III)*

PB17* **Ovad, T.**: *Electron force field as a gateway to X-ray photochemistry?*

PB18 **Pluhařová, E.**: *Structure and dynamics of concentrated dextran solutions by molecular dynamics simulations*

PB19* **Salomon, J.**: *Temperature-Dependent Conformational Equilibrium of RNA 2'-OH Groups in Molecular Dynamics*

PB20 **Sawicki, I.**: *Improving the performance of Double Hybrid functionals through regularization*

PB21 **Malček Šimunková, M.**: *Redox Behavior and Biomolecular Targeting of Acacetin-Cu(II) Complex: A DFT, Spectroscopic and Molecular Modeling Approach*

PB22 **Sit, M.**: *Excited State Molecular Dynamics Simulation of Silaethylene including Spin-Orbit Coupling*

PB23* **Skladanová, K.**: *Isobutanol to 2-butoxide on (100) surface of ferrierite: Insights from ML-accelerated AIMD*

PB24 **Štekláč, M.**: *Structure-Based Identification of Musky Odorant Ligands Targeting Human Olfactory Receptor 5A2*

PB25 **Sujkowski, E.**: *The Reversal Spin-Flip (RSF) ApproachWithin pCCD for Open-Shell Quantum State*

PB26 **Šulka, M.**: *Analyzing the nature of electron correlation in small metal clusters*

PB27 **Šulková, K.**: *Superalkali Clusters for CO_2 Activation: Role of Electronic Structure, Surface Charges and Ionization Potential*

PB28 **Świerczyński, J.**: *Overcoming Bottleneck Operations in the Molecular Property Calculations in PyBEST with GPUs*

PB29 **Tokárová, Z.**: *Electronic structure of small organic molecules: DFT insights compared to experimental results*

PB30 **Tsuru, S.**: *Equation-of-motion coupled cluster theory for describing arbitrary conical intersections*

PB31 **Tyrcha, B.**: *Recent developments in second-quantization-based symmetry-adapted perturbation theory*

PB32* **Uhliar, M.**: *On the influence of halogen substitution on aromaticity in benzene-based systems*

PB33* **Witkowski, M.**: *Ultrafast correlation energy estimator*

PB34* **Zajaček, D.**: *Implicit solvation models as an alternative for estimation of Clog P coefficient*

Invited Lecture Abstracts

An Evaluation of the Hybrid KS DFT Functionals Based on the KS Exchange-Correlation Potentials

Vignesh Kumar, Szymon Śmiga and Ireneusz Grabowski

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We have developed a methodology for the evaluation of the quality of hybrid exchange-correlation (XC) density functional approximations (DFAs) based on very fundamental quantities, i.e., Kohn−Sham (KS) XC potentials, self-consistent electron densities, first ionization potentials (IPs), and total energies. Since the XC potentials, the primary objects in the current study, are not directly accessible for the hybrids, we calculate them by inverting the KS electron densities. Utilizing this methodology, we tested 155 hybrid DFAs available in the LIBXC library using FCI and CCSD(T) methods as a reference. [1]
We have found that a group of functionals produces very decent XC potentials, mainly those with a large mixture of Hartree−Fock exchange. Moreover, the value of IP strongly depends on the XC potential quality. On the other hand, we show that the XC energy is dominated by functional-driven error, which in some cases leads to substantial errors in electronic densities. In addition, we offer that the CCSD(T) method is a sufficiently quantitative reference for this type of evaluation without the need to use expensive FCI calculations. The study shows new directions for constructing more accurate XC functionals within the KS-DFT framework and evaluating the existing ones. [2]

References

[1] V. Kumar, S. Śmiga, I Grabowski, https://doi.org/10.18150/V4XZSF

[2] V. Kumar, S. Śmiga, I Grabowski, J. Phys. Chem. Lett. 2024, 15, 10219−10229

Going beyond standard DFT in periodic systems: the story of fluorographene

Petr Lazar,[1]* Vítězslav Hrubý,[1] Miroslav Medveď,[1,2] Giorgio Zoppellaro[1,3] and Michal Otyepka[1,4]

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Fluorographene, a monolayer form of carbon monofluoride, is a fluorinated graphene derivative with intriguing properties. Unlike graphene, fluorographene is a wide gap semiconductor/insulator that holds great potential for applications requiring two-dimensional dielectric nanomaterials. Despite its simple structure, even the basic question of fluorographene's band gap size was a long-standing conundrum because its values from various theoretical frameworks from standard DFT to many-body perturbation theory differed wildly [1].

This talk will illustrate applications of DFT and current beyond-DFT methodologies (GW, Bethe-Salpeter equation) to diverse properties of fluorographene. We will attempt to highlight where the methods work, where they fail, and what are the current limits in application of beyond-DFT methods in periodic solid-state systems. We also report how advanced ab initio calculations were instrumental in demonstrating that polarons are formed at the radical sites in fluorographene [2] and, by that, providing a comprehensive scenario for an unexpected phenomenon of solvent-induced generation of polaronic spin active states in fluorographene under UV light [3].

References

[1] V. Hrubý, L. Zdražil, J. Dzíbelová, V Šedajová, A. Bakandritsos, P. Lazar, M. Otyepka, *Appl. Surf. Sci.*, *587*, *152839 (2022).*

[2] M. Medved, G. Zoppellaro, J. Ugolotti, D. Matochova, P. Lazar, T. Pospisil, A. Bakandritsos, J. Tucek, R. Zboril, M. Otyepka, *Nanoscale 10, 4696 (2018)*

[3] G. Zoppellaro, M. Medveď, V. Hrubý, R. Zbořil, M. Otyepka, P. Lazar, *J.Am. Chem. Soc. 146 (22), 15010 (2024)*

Isobutanol conversion catalyzed by acidic zeolites

Monika Gešvandtnerová,[1,2]* Michael Badawi,[2] Céline Chizallet,[3] Pascal Raybaud,[3] Tomáš Bučko[1,4]

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Computational investigations play an increasingly important role in the study of solid-state materials, as they enable understanding of the observed rectivity and energetics, prediction of new structures and mechanisms, and, in general terms, provide access to atomistic details that are not easily accessible in experiment. Experimental studies have revealed that zeolite ferierite exhibits a high selectivity for conversion of isobutanol to linear butenes [1,2]. However, despite the high technological potential in the field of sustainable fuel production, the reaction mechanisms are not yet fully understood, hindering the optimization of more efficient solid- state catalysts. In our previous static theoretical study [3], based on periodic DFT calculations, we have revealed a network of monomolecular transformations of butanols to butenes catalyzed by framework bridging OH groups in model zeolite chabazite. We identified previously unexplored transformation pathways involving isobutanol isomerization followed by dehydration as dominant at relevant experimental conditions. While the static approach, based on statistical mechanics approximation, enables quantitative analysis, its accuracy is insufficient for realistic predictions [4] of rate constants. To overcome these limitations, we employed Blue moon ensemble *ab initio* molecular dynamics (AIMD) with path-based reaction coordinate [5] and Bennett-Chandler theory to study the key reaction mechanisms of isobutanol to butene transformations. In addition to isobutanol isomerization, identified as the key step of the dominant pathways leading to linear butenes and isobutene, the competing pathways for direct isobutanol to linear butene and isobutanol to isobutene transformations were studied. AIMD results revealed that the competing pathways for isobutanol to linear butenes transformation share a common dynamical transition state [6]. For the case of isobutanol to isobutene transformation, the common dynamical transition state was found to be shared between the key step and a previously unexplored transformation pathway involving synchronous dehydration and isomerization. The preference for synchronous isomerization and dehydration pathway was found to increase with higher temperature, with the product formation determined by fine details, such as specific atomic positions and momenta, that are subject to essentially random fluctuations during the diffusive motion of water.

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Electronic Structure Insights into Reactivity Across Ground and Excited States in Nickel Photocatalysts

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Ni(II)–bipyridine aryl halide complexes have emerged as broadly useful photoactive pre-catalysts in cross-coupling reactions, where visible light promotes Ni–C(aryl) bond homolysis to generate reactive Ni(I) species.[1] Despite recent progress, questions remain about the excited states involved and how ground-state electronic structure influences downstream reactivity.

We combine computations, synthesis, and spectroscopy to address these questions. Time-dependent DFT and multireference methods (CASSCF/NEVPT2) are employed to map the excited-state landscapes of these complexes and to reveal that dissociative ligand-to-metal charge transfer (LMCT) states are key in promoting Ni–C bond homolysis upon photoexcitation. Systematic tuning of bipyridine and aryl substituents analyzed via Hammett correlations and charge-transfer energetics shows how ligand electronics control this process.[2]

We further explore a geometrically constrained (tethered) Ni(II) complex, where ligand rigidity stabilizes a reversible [Ni(I)…aryl$^{\bullet}$] contact pair in the excited state. Transient absorption spectroscopy supports the computed excited-state behavior and underscores the impact of structural constraints on photoreactivity.[3]

To probe downstream reactivity, we analyze the electronic structure of Ni(I)–bipyridine halide species. The energy of the Ni 3d(z^2) orbital emerges as a key ground-state descriptor, correlating with both productive oxidative addition and off-cycle dimerization pathways. This finding provides a predictive handle for tuning Ni(I) reactivity via ligand design.[4]

Overall, our integrated approach connects excited-state dynamics and ground-state reactivity, offering design principles for more effective photoactive nickel catalysts.

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Methods for simulating excited-state dynamics in complex systems and environments

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Simulating excited-state dynamics in complex systems presents a fundamental challenge: the quantum many-body problem scales exponentially with system size, rendering exact solutions computationally intractable for realistic systems. Yet, understanding these dynamics — from energy transfer in photosynthetic antennae to emergent phenomena in polaritonic materials — demands theoretical approaches that carefully balance accuracy with computational feasibility. In this presentation, I will present some strategies to address this challenge. First, I will present the formulation and implementation of a "divide and conquer" strategy based on exciton models within mixed quantum-classical dynamics, which enables the study of excited-state dynamics in multichromophoric systems in complex environments.[1, 2, 3] In the second part, I will discuss innovative strategies for polaritonic chemistry, where photons are treated as classical "extra degrees of freedom".[4] This approach enables the integration of photons into trajectory-based methods, offering a significant potential to advance the study of organic exciton-polaritons. Finally, I will show how combining quantum and classical computers can help simulate excited dynamics in molecules.[5]

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Machine Learning Surrogate Models of Electronic Structure for Quantum Dynamics and Inverse Design

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Atomistic simulation based on quantum mechanics (QM) is currently being revolutionized by machine-learning (ML) methods. Many existing approaches use ML to predict molecular properties based on quantum chemical reference data. This has enabled molecular property prediction within vast chemical compound spaces and high-dimensional parametrization of energy landscapes for the efficient simulation of measurable observables. However, as all properties derive from the QM wave function, an ML model that can predict the wave function or the electronic Hamiltonian also has the potential to predict other properties. In this talk, I will explore ML approaches that deliver surrogate models of the electronic structure based on electronic structure Hamiltonians with the aim to develop methods that use ML and QM in synergy. Using example systems from heterogeneous catalysis and organic electronics, I will discuss the challenges associated with encoding physical symmetries and invariance properties into linear and deep learning mappings of atomic configuration and composition onto electronic structure. Upon overcoming these challenges, integrated ML-QM methods within modern, modular software frameworks offer the combined benefits of data-driven parametrization and first-principles-based methods. I will discuss several opportunities associated with building ML-augmented quantum chemical methods, including Inverse Chemical Design based on ML-predicted wave functions and the development of efficient and accurate surrogate models to study materials chemistry.

Nature counts to three: Universal Mg-pinch motif polarizes the cleaved bond in NTP-processing enzymes

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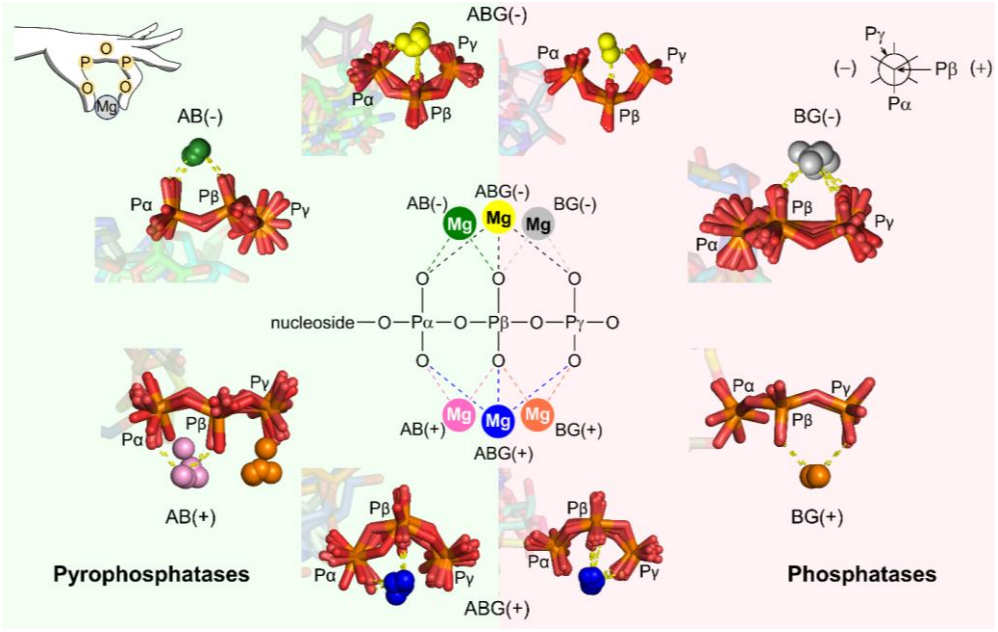
The formation and cleavage of phosphate bonds are essential in most biological processes including nucleic acid processing. Many enzymes that catalyze phosphate hydrolysis require bound divalent metal ions. Most commonly, Mg^{2+} ions are required for catalysis, while similar Ca^{2+} ion abolishes the catalytic activity. To elucidate the often controversial mechanism of these ubiquitous metal ion catalyzed reactions, we carry out hybrid quantum-classical QM/MM free energy simulations. Curiously, Nature uses nucleoside triphosphates (NTPs) for the myriad enzymatic reactions involved in all life processes. The enzymes that deal with four or more phosphates are outnumbered by NTP catalytic proteins. Additionally, NTP is broken down to NMP or NDP, freeing up (or transferring) a pyrophosphate or a phosphate, respectively. In less than 10% of cases, all three phosphates are removed. We propose a universal Mg-pinch motif within NTP-catalytic enzymes and provide a comprehensive overview of all structural patterns currently discovered for NTP catalysis, delineating the key role of the Mg^{2+} ions in polarizing phosphate groups.



Basis-set limit MP2 correlation energies for large molecules

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We present an integral-direct, iteration-free, linear-scaling, local explicitly correlated second-order Møller–Plesset (MP2-F12) approach, which additionally proves efficacious for the evaluation of perturbative terms within double-hybrid density functionals. The methodology is predicated upon a fragmentation approximation: correlation contributions for individual electron pairs are computed within domains defined by their corresponding localized orbitals, while the correlation energies of spatially distant electron pairs are determined via multipole expansions. The requisite electron repulsion integrals are computed directly employing the density fitting approximation, thereby precluding the need for integral and intermediate storage. Furthermore, the approach leverages compression techniques to diminish the dimensions of the density fitting and resolution of identity auxiliary basis sets associated with these domains, consequently reducing operation count and memory footprints. Validation studies indicate that this approach recovers at least 99.9 % of the canonical MP2-F12 correlation energy and yields reaction energies with a mean absolute error of 1 kJ/mol. A comparative analysis of the approach's performance against alternatives, including basis set extrapolation and density-based basis set correction, is also presented.

From relativistic spectroscopy to quantum electrodynamics and back

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A new way of doing chemistry has recently been proposed based on optical cavities – nanostructures that confine light and promote strong coupling between quantized cavity modes and embedded matter. This strong coupling leads to the formation of mixed light–matter states, known as polaritons, which modify molecular excited-state landscapes. As a result, it becomes possible to control chemical reactions, influence transport processes, and even induce new states of matter. Due to the quantized nature of light, the theoretical description of such systems must be grounded in quantum electrodynamics (QED), the fundamental theory of electrons and photons. Furthermore, accurately capturing the effects of strong coupling on matter requires combining first-principles quantum chemical methods with a treatment of photons as dynamical variables.

In this talk, we will present relativistic quantum electrodynamical density functional theory (QEDFT) based on the four-component Dirac–Coulomb [1] and two-component X2C Hamiltonians [2]. The theory is derived from first principles and yields equations that provide spectra and transition properties of strongly coupled electron–photon systems. The method has been implemented in the relativistic spectroscopy program ReSpect [3], extending the program's functionality from purely electronic systems to coupled electron–photon systems. Owing to its relativistic nature, the developed method can describe cavity-induced modifications of properties of heavy-element-containing molecules, including processes driven by spin–orbit coupling that are formally forbidden in non-relativistic theories. The two-component version further reduces computational cost while preserving accuracy, enabling the study of large molecules and collective coupling effects in molecular ensembles. Finally, we will demonstrate that QEDFT, originally developed for matter in optical cavities, can also be applied to describe spectroscopic phenomena arising from coupling to the quantum vacuum, such as spontaneous emission and the Lamb shift. Thus, we extend the reach of relativistic spectroscopy into the domain of cavity QED while at the same time also bring new physical insights from light–matter interactions back into the realm of molecular spectroscopy.

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Ultracold highly magnetic and polar molecules for quantum simulation and new physics search

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Ultracold mixtures involving highly magnetic atoms such as Er+Li, Dy+K, Cr+Li, and Er+Yb have already been realized for studying exotic quantum many-body phases. Such mixtures also open the way for the formation of ultracold diatomic molecules having both significant magnetic and electric dipole moments. Molecules involving atoms with large orbital angular momenta, such as Dy and Er, have a prohibitively complex internal structure with chaotic rovibrational spectra. In contrast, molecules involving highly magnetic symmetric atoms such as Cr or Eu may form exotic doubly polar molecules with easier-to-predict structures. On the other hand, molecules involving electronegative coinage metals such as Ag and alkali-metal atoms should possess very large permanent electric dipole moments.

In my talk, I will present several classes of highly polar and paramagnetic diatomic molecules, which can be produced at ultralow temperatures from laser-cooled ultracold atoms. I will show a new mechanism of useful Feshbach resonances in Cr+Yb mixtures [1] and the application of ground-state YbCr molecules for new physics searches [2], a recent experimental realization of weakly-bound LiCr molecules and our theoretical prediction of transferring them to the absolute ground state [3], as well as all-optical formation schemes of highly polar KAg and CsAg molecules [4]. Finally, I will discuss the possible application of ultracold highly polar and paramagnetic diatomic molecules in studying controlled collisions and chemical reactions and using them for precision measurements, quantum simulations, and quantum computing.

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Tunneling splittings in vibrational spectra of molecules using modified WKB in Cartesian coordinates

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In molecular systems with multiple equivalent symmetry-related minima separated by potential barriers, vibrational states can delocalize over the entire system via tunneling. This phenomenon manifests itself in the energy splittings of the delocalized states in vibrational spectra. Tunneling splittings vary over many orders of magnutide depending on the type of rearrangement involved and modal excitations of the system. Calculation of tunneling splittings using variational methods for molecules larger than a few atoms is computationally prohibitive. We present a semiclassical theory for calculating tunneling spectra that is scalable to larger systems in full dimensionality.

The method is based on a modified WKB theory in which an approximate wavefunction is constructed along the minimum action paths that connect the symmetry-related minima [1, 2]. We show that the approach is equivalent to the instanton theory for tunneling splittings of the ground vibrational state and that it gives an exact wavefunction in a harmonic potential for the ground and the first excited state. We test it on vinyl radical [3] and malonaldehyde [4] and apply it to calculate tunneling splitting in larger systems, the formic acid dimer and the water hexamer [5] in the ground and vibrationally excited states. We also present an extension to estimate the splittings of rotationally excited states in HO_2 molecule and discuss future directions with a view of calculating tunneling rates in molecules at low temperatures.

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Application of Free Energy Perturbation in Structure-Based Drug Design: Insights from Adenosine Receptors

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Accurately predicting changes in binding free energy is essential for linking structural modifications—whether in ligands or receptor mutations—to observed experimental binding affinities. Free energy perturbation (FEP) methods have long been used to explore structure–affinity relationships, and recent advances now allow their routine application in structure-based drug design. In addition to ligand optimization, these methods can be applied to evaluate the impact of site-directed mutagenesis, further supporting predictions of binding modes. By combining ligand and residue FEP simulations, it is possible to generate detailed energetic maps of protein–ligand interactions. To facilitate this, our group has developed two complementary protocols—QligFEP [1] and QresFEP [2]—implemented within the Q molecular dynamics software.

Adenosine receptors (A_1, A_{2A}, A_{2B}, and A_3) are G protein-coupled receptors (GPCRs) that mediate cellular responses to extracellular adenosine, playing important roles in processes such as inflammation, immune regulation, and the sleep–wake cycle. Among them, the A_{2A} and A_{2B} adenosine receptors (A_{2A}AR and A_{2B}AR) have emerged as promising therapeutic targets due to their upregulation under pathological conditions such as cancer, where elevated adenosine levels suppress immune activity within the tumor microenvironment.

In this lecture, I will present several case studies where FEP methodology has proven highly valuable in the rational design of ligands and in elucidating structure–activity relationships for A_{2A}AR and A_{2B}AR ligands [3]. I will also highlight a specific example in which the application of FEP helped resolve the precise binding mode of the selective A_{2B}AR agonist BAY60-6583. This ligand had been crystallized in two alternative orientations, raising uncertainty about its physiologically relevant binding mode. By applying a combination of ligand and residue FEP approaches, we were able to clarify this ambiguity and establish a solid foundation for the design of next-generation selective A_{2B}AR agonists [4].

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Contributed Talk Abstracts

Metal-metal interactions in an open d-shell system with cuprite structure

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Cuprite is one of the most studied *p*-type semiconductors and an extremely attractive low-cost material for sustainable energy application [1]. Its crystal structure is characteristic for suboxides of the Group 10 elements with a closed valence nd^{10} shell. Due to the technological importance and intriguing nature of the cuprite structure, which consists of interpenetrating 'closed-shell' M-O sublattices, the chemical bonding in these compounds has been intensively investigated [2, 3]. The role of the metal-metal, resp. cation-cation interactions have been particularly discussed while partial depopulation of the metal *d* shell and the formation of multicentre metal-metal bonds have been invoked. However, a study, which would particularly focus on the impact of an open *d* shell on metal-metal bonding in the cuprite structure and specifically on the formation of multicentre metal-metal bonds is missing.

In our study, the formation of directional metal-metal interactions and multicentre bonds is for the first time revealed in a cuprite structure of Pd_2O with a partially open *d* shell employing Density Functional Theory with evolutionary algorithms for crystal structure prediction. This study presents the first detailed description of Pd(I)-Pd(I) bonding in an inorganic compound. Simultaneously, it brings important new insight into the discussion of metal-metal bonding in technologically very important cuprite compounds. This study also presents an important contribution to the inorganic chemistry of Pd(I) compounds, which is an uncharted territory, currently limited to the delafossite compounds $PdMO_2$ (M = Co, Cr, Rh) with extremely mobile Pd *d* electrons and Pd_2O, which remains uncharacterized [4].

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Theoretical Exploration of HER Mechanisms on Transition Metal Phosphide Surfaces

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Transition metal phosphides (TMPs) are increasingly recognized as a class of highly active, stable, and cost-effective catalysts for the hydrogen evolution reaction (HER), offering a viable alternative to scarce and expensive platinum-group metals. Their unique structural characteristics, featuring metal-phosphorus bonds that promote charge delocalization and optimal hydrogen binding, enable efficient proton reduction across a wide pH range. Among TMPs, systems based on Mo, Ni, and Fe exhibit promising bifunctional properties, and their catalytic behavior can be finely tuned through doping, defect engineering, and facet control. However, a deeper theoretical understanding of the surface-dependent HER mechanisms is essential for rational catalyst design.

In our research, we combine density functional theory (DFT) simulations with experimental analysis to investigate the HER performance of MoP, Ni-P, and Fe-P catalysts. Using slab models of MoP(101), (110), and (100) surfaces, and P-modified Ni(111) and Fe(110) surfaces, we computed hydrogen and water adsorption energies, Gibbs free energies of hydrogen adsorption (ΔG_{H^*}), and charge density distributions. The calculation of ΔG_{H^*} was based on the computational hydrogen electrode model proposed by Nørskov et al. [1], which enables a quantitative assessment of HER thermodynamics. Our results demonstrate that MoP(101) and MoP(110) facets provide favorable adsorption environments for H_2O and H*, with ΔG_{H^*} values supporting high HER activity in alkaline media [2].

Similarly, Ni(111) surfaces modified with P atoms showed near-ideal hydrogen adsorption characteristics ($\Delta G_{H^*} \approx 0.01$ eV), correlating with experimental Tafel slopes as low as 79 mV dec^{-1} and enhanced electrochemical surface area ($C_{dl} \approx 42$ mF cm^{-2}). By contrast, Fe(110) surfaces modified with P atoms exhibited stronger hydrogen binding ($\Delta G_{H^*} \approx -1.32$ eV), which may hinder desorption and limit HER kinetics. Theoretical insights were validated through polarisation curves, impedance spectroscopy, and stability tests, confirming the superior catalytic performance of MoP and Ni-P foams in alkaline environments. This work highlights the utility of first-principles simulations in interpreting complex electrochemical behavior and provides a computational framework for tailoring TMP catalysts through atomistic surface engineering.

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DFT INSIGHTS INTO DEFECT AND TEMPERATURE-DEPENDENT BAND GAPS IN HALIDE PEROVSKITES

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The optical transitions in active layers of halide perovskite's (PV) films crucially determine their optical absorption properties to a large extent. Sub-bandgap absorption of incident photons in the PVs absorbers can result either from structural imperfections or from thermal disorder [1,2]. These factors could influence the charge recombination processes, which play a significant role in restricting the performance of perovskite-based applications in photovoltaics.

We will demonstrate methodology based on exchange-correlation approaches of Density Functional Theory (DFT) exploited in simulations of exciton binding energy comparable with experimental data [3]. By DFT modelling in the PAW approximation we investigated the development of electronic bands and trap states of hybrid PV $MAPbI_3$ with the increasing concentration of Pb/I vacancies in the modelled crystal structure, underlying physics of defects and lattice dynamics. We will also briefly present the developed statistical procedure for computation of electron-phonon coupling [4] resulting in the observable temperature dependence of band gap in example inorganic PV $CsPbI_3$ crystal. The simulated behaviour of electronic gap dispersion is related to Urbach energy parameter describing sub-bands from optical measurements of PV structures [5]. Described DFT procedure in conjunction with a quasi-harmonic lattice dynamics could represent a viable interpretation not only to electro-optical measurements but should be extendable to support the effective fabrication techniques of photovoltaic devices based on grown PV films.

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Simplified, Physically Motivated, and Broadly Applicable Range-Separation Tuning

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Range-separated hybrid functionals developed within the Kohn-Sham Density Functional Theory (DFT) are quite often coupled with ionization energy tuning or optimal tuning of the screening parameter [1] strategies to boost their predictive power. These kinds of functionals are widely recognized as accurate and effective tools for modeling excited-state behavior in various systems, including condensed-phase matter. However, these techniques typically require iterative self-consistent calculations, which can be computationally expensive and potentially unstable-particularly in large-scale systems.

In this study [2], we propose a simple and efficient alternative for determining the screening parameter, based solely on the system's total electron density and the compressibility sum rule from DFT . The resulting parameter exhibits excellent accuracy, especially for charge-transfer excitations, and outperforms previously established methods [3]. By solely relying on the electron density, the approach offers a clear theoretical foundation and is easily adaptable to automated DFT workflows in complex or bulk systems, where conventional tuning strategies are impractical.

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Actinide-actinide bonding in fullerenes. A challenge for theory

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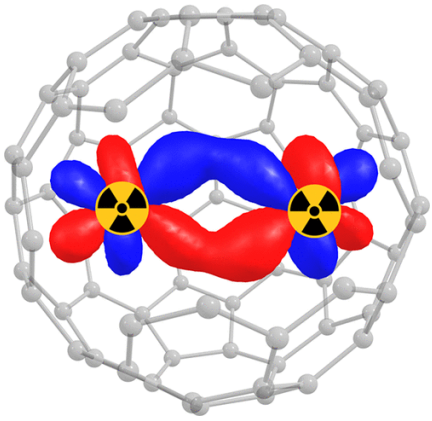
Actinide-actinide bonding poses a challenge for both experimental and theoretical chemists because of both the scarcity of experimental data and the exotic nature of actinide bonding due to the involvement and mixing of actinide 7s-, 6p-, 6d-, and particularly 5f-orbitals. Only a few experimental examples of unsupported An–An bonding have been reported so far, e.g. in U_2 and Th_2. Recent theoretical prediction[1] and experimental characterization[2] of the $U_2@C_{80}$ opened the avenue for actinide–actinide bonding in fullerene cages. In 2020 we predicted existence of An-An bonding inside various fullerene cages such as, C_{70}, C_{80}, C_{90} along the Ac-Cm actinide series using DFT BP86.[3] Later, we unraveled an enormous dependence of the DFT-calculated An–An bond order (expressed via delocalization index from QTAIM analysis) on the DFT functional used.



Here, I will present a methodological study[4] of actinide-actinide bonding on experimentally known $Th_2@C_{80}$ and $U_2@C_{80}$ systems. We compared selected GGA, meta-GGA, hybrid-GGA and range-separated hybrid-GGA functionals with the results obtained using multireference CASPT2 method, which we consider as a reference point. We show that GGA functionals perform well for predicting geometries, while range-separated hybrids are superior in the description of the chemical bonding. None of the tested functionals were deemed reliable regarding the correct electronic spin ground state. Based on the results of this methodological study, we re-evaluated selected previously studied diactinide fullerene systems using more reliable protocol.

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Electronic Transitions in Supramolecular Aggregates

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Multichromophoric systems are ubiquitous in nature (e.g., DNA molecule, photosystems in chloroplasts, etc.) and they also play inevitable role in the design of materials with various applications, such as photovoltaics, photocatalytic systems, OLEDs, etc. However, it is inconvenient to study their electronic spectra and properties with conventional electronic-structure methods, due to their size.

In this talk, I will present the advancements in the development of excitonic configuration interaction (ECI) method[1] and its implementation in the SHARC package.[2] ECI efficiently calculates electronic states of multichromophoric systems in the exciton style – it calculates each chromophore separately on a desired conventional level of theory (so-called site-state calculations), builds a basis of antisymmetrized products of the site states (excitonic basis), builds the full-system Hamiltonian in the excitonic basis within the strong-orthogonality assumption, and diagonalizes it. If combined with the resolution-of-identity (RI) approach, ECI effectively scales linearly with the number of chromophores.[3] Its performance in calculating absorption electronic spectra will be illustrated on a series of supramolecular clusters extracted from the crystal structures of various organic solids, with individual chromophores being treated at the TD-DFT and EOM-CCSD levels. It will be shown that the method can accurately handle the clusters of sufficient size to reproduce bulk features, such as electronic bands instead of line spectra (as characteristic for small molecular systems).

I will also discuss prospects of connecting ECI with the SHARC approach[4] to the non-adiabatic dynamics, which would enable real-time simulations of ultrafast energy-transfer processes in multichromophoric systems, such as Förster resonance energy transfer, Dexter energy transfer, singlet fission, and charge transfer.

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Intermolecular-type conical intersections in molecular dimers

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So far, the search for conical intersection (CI) type geometries in molecules has been almost exclusively limited to individual monomers analysis. Recently, in the case of catechol [1] and benzene [2] molecules, it has been shown that these CI geometries can be formed not only within monomers, but also in dimeric systems. Surprisingly, the resulting dimer-type CI geometries are energetically similar to, and perhaps even more favorable than, the monomer-type CIs known so far. However, to accurately identify these CI geometries, theoretical methods are needed that take into account not only static (or multireference) electron correlation effects, but also the higher-order correlation effects such as the dispersion interaction between monomers. Accordingly, the equilibrium geometries of the ground and first electronic excited states as well as the radiationless deactivation channels of catechol and benzene in their monomer and dimer configurations were investigated using the standard linear-response and the spin-flipped TDDFT together with the ωB97X-D3 exchange-correlation functional, as well as by the multireference CASSCF methods, considering the minimally augmented ma-def2-TZVPP and the 6-31G** basis sets. It was found that for the equilibrium geometry the stacking distance between the monomers decreases in the first electronic excited state, due to the stronger intermolecular interaction energy, bringing the two monomers closer together. Intermolecular-type CI geometries can be formed between the two monomers, where both aromatic rings show planar deformation and a weaker, approximately 1.6–1.8 Å long, C–C bonds are formed between the two monomers, with multiple orientation configurations of the monomers relative to each other. It was also shown that, these, intermolecular-type CIs are energetically more favorable than CIs containing only one deformed monomer. The validity of the dimer-type CI geometries obtained by SF-TDDFT was confirmed by the CASSCF method.

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Towards accurate simulations of the optical signatures of fluorophores

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There is a very high demand for the development of improved fluorophores which are, e.g., essential for advancing our understanding of biological processes. However, the optimization of fluorescence is typically performed with a trial-and-error synthetic approach that is costly and generates waste. Therefore, our study focuses on employing quantum chemical calculations as a more effective approach to drive the experimental developments toward the most desirable dyes. In this context, the ultimate object of this research is to deliver a quantum-chemistry protocol enabling accurate prediction of two essential features of the fluorophores that are currently hardly evaluated, the emission quantum yield and brightness. To this end, we are employing a Fermi Golden rule approach for the radiative and internal conversion rates and include the impact of minimum energy conical intersections in the calculation.[1]

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Cu(I)-based heteroleptic photosensitizers – a theoretical analysis of the low-lying excited states

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Heteroleptic Cu(N^N)(P^P) complexes are used as photosensitizers in various processes, ie. in dye-sensitized solar cells [1], organic light emitting diodes [2] or photocatalysis, in particular in the $CO_2 \rightarrow CO$ reduction reaction. For the last purpose they can be seen as the promising, more environmentally friendly and more feasible successors of well-known noble metal-based photosensitizers, in which cations of metals such as ruthenium, rhenium or iridium play the role of the central metal. Even though such systems have been synthesized, and their photocatalytic activity has been confirmed [3], not much is known about the mechanism of photosensitization. To gain in-depth insight into this topic, quantum chemistry methods need to be employed. Owing to the considerable size of the Cu(I)-based diimine-diphosphine photosensitizers, the applicable theoretical methods are limited to DFT-based ones. Their characteristics, however, such as extended regions of π-electron delocalization as well as considerable CT character of the low-energy excited states render them particularly troublesome for DFT. Hence, a thorough methodological study to establish a proper computational protocol had to be performed first. Optimal approach was selected based on comparisons with available experimental data as well as with other computational approaches applied to simplified model systems.
A series of Cu(I)-based diimine-diphosphine complexes with varying diimine ligands are characterized. Particular attention is paid to the low-lying singlet and triplet states, which play the crucial role in the photosensitization process. We characterize their energetics, especially with respect to the Cu-center conformation, and analyze in detail their character based on difference densities and on the 1-electron transition density matrix formalism (as implemented in TheoDORE [4]).

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Study of Photorelaxation Pathways in 7H and 9H tautomers of 2,6-Diaminopurine

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Understanding the ultrafast relaxation mechanisms of photoexcited nucleobase analogs is crucial for elucidating their photostability and potential biological implications. In this study, we employ nonadiabatic molecular dynamics simulations with surface hopping to investigate the ultrafast relaxation mechanisms of 2,6-diaminopurine in both its 7H and 9H tautomeric forms. Simulations are performed in vacuum and aqueous solution (implicit water clusters) using DFT/TDDFT electronic structure. Our results highlight the influence of solvation and on the excited-state dynamics and the role of conical intersections in system relaxation back to the ground state. This study provides deeper insights into the photophysics/photochemistry of purine derivatives and their implications for photostability in biological and biomimetic systems.

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Comparison of interactions of proteins with poly(ethylene oxide) layers in two setups

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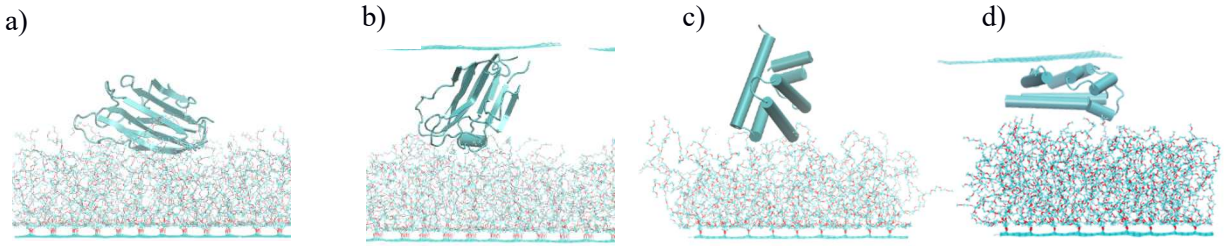
A comprehensive understanding of the interactions between proteins and biomaterial surfaces is essential for the development of various biomedical applications, including drug and gene delivery systems, implants biosensors, and bioassays. The undesired nonspecific adsorption of proteins onto biomaterials can impair their performance, often triggers an immune response, and may also induce protein denaturation [1, 2]. Currently, the most effective method to mitigate protein adsorption on material surfaces is to coat them with a layer of hydrophilic and biocompatible polymers represents nowadays most efficient way to prevent adsorption of proteins on material surfaces. Experimental techniques typically investigate the interactions of free proteins with these polymer layers or utilize setups where a protein is anchored to a tip or surface that is pushed against the polymer layer by an external force. However, the conditions employed in the latter setup mimicking atomic force microscopy (AFM) do not accurately reflect the conditions found in biological systems due to the steric and entropic constraints introduced. This raises concerns about whether the restricted conditions experienced by proteins may inaccurately suggest protein repulsion from the polymer layer, even when free proteins exhibit attractive interactions. Atomistic molecular dynamics simulations were performed to compare these two considering poly(ethylene oxide) (PEO) as a widely used coating material. The effect of different grafting densities, σ, of PEO chains giving rise to the formation of pancake, brush, and extended brush conformations of the PEO layer was studied. The conformational response of two proteins, characterized by predominant α-helices and β-sheets in their secondary structure, were compared. It was discovered that under specific conditions, the two setups yield differing conclusions regarding adsorption. An explanation for this discrepancy was provided.



PEO layer grafted on graphene at $\sigma = 1.6$ nm^{-2} interacting with a free fragment of the C1q protein characterized by a predominance of β-sheets (a) as well as with a C1q fragment anchored to a tip that mimics AFM conditions (b). PEO layer grafted on graphene at $\sigma = 1.6$ nm^{-2} interacting with a free fragment of human serum albumin, which is mainly composed of α-helices (c) and with a human serum albumin fragment anchored to a tip mimicking the AFM conditions (d).

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Modeling the uptake of small oxidized organic molecules by gas-phase hydrated nitric acid clusters

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Aerosol particles are suspensions of solid or liquid particles in air. Apart from water, they contain more complex molecules such as inorganic acids or various organic compounds. They are a key component of atmosphere, functioning as heterogeneous catalyst and influencing various processes, such as the greenhouse effect. In polluted areas, they have been found to severely impact human health. Despite previous extensive studies, the initial steps of their formation at a molecular level are still unknown [1, 2]. This *new particle formation* can be mimicked by experiments utilizing molecular beams [1]. However, to understand the detailed mechanism on a molecular level, methods of computational chemistry have to be used.

This study focused on uptake of carboxylic acids (formic acid and acetic acid) and aldehydes (formaldehyde and acetaldehyde) on hydrated nitric acid clusters. We collected and analyzed tens of thousands independent classical molecular dynamics trajectories of the organic molecule – cluster encounter. We identified various processes, such as sticking collision or direction change, provided details of non-bonding molecule – cluster interactions and estimated the pickup cross sections and their dependence on the oxidation state of the molecule as well as its size. Our previous study [3] of the pickup of alcohols showed exceptional agreement of the relative pickup cross section of the alcohols with experimental data. The present study of more oxidized molecules identified limitations of the computational setup. Overall this work provides better understanding of the formation of aerosol particles.

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Super-reduced metals in enzymes: why and how? The case of cobalamin and coenzyme F_{430}

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In this study we focused on three protein cofactors, all of whom possess a characteristic tetrapyrrole ring that coordinates to a central metal atom: corrin, found in vitamin B_{12}, corphyn, found in cofactor F_{430}, and porphyrin, found in heme, the key component of hemoglobin [1]. The reaction mechanism of cobalamin within the enzyme methionine synthase (MTR) [2] is characterized by the metal center of cobalt employing a remarkable electron configuration of Co(I), with a fully occupied d_{z2} orbital. A similar situation is found in cofactor F_{430}, which employs a super-reduced state for nickel [3]. Interestingly, the related metal-porphyrin complexes such as heme are not known to engage in super-reduced states in any protein under physiological conditions [4]. In this regard, there is an interesting potential in understanding the choices made by the proteins that operate via super-reduced metal states, and in discovering other super-reduced states, in order to elucidate further enzyme reaction mechanisms, as well as deepening our understanding of the current way in which enzymes operate.

Thus, we have performed QM calculations with detailed analyses of the molecular orbital landscapes on four tetrapyrrole ring analogues, where the central atom is substituted by other third-row transition metals, such as cobalt, iron, manganese, and nickel in the +1 formal oxidation state and with various spin configurations. Then, we performed QM/MM calculations on full models of the F_{430} cofactor and its respective MCR enzyme in order to observe the degree to which the protein would accommodate a super-reduced metal, and the stability of the super-reduced state of the metal within the enzyme. Rationales for the distinct choices of cobalt in vitamin B_{12}-dependent methyl transferases vs. nickel in the F_{430}-dependent methane-synthesizing enzyme MCR are derived for the first time from these calculations.

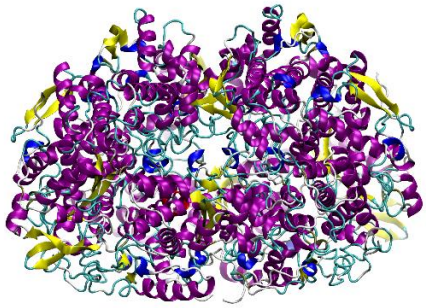

Figure 1. Crystal structure of the MCR enzyme (PDB: 7B1S), at 0.99Å

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Single-reference coupled cluster theory for systems with strong correlation extended to excited states

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Coupled cluster (CC) theory [1,2] has size-extensivity and is regarded as "gold standard" of electronic structure theory based on wave functions. Nevertheless, conventional CC theory referenced to a single Slate determinant is troublesome for systems with strong correlations due to instability of the reference. Although multireference (MR) CC is simple idea as adaptation of CC theory to systems with strong correlations, some technical difficulties inherent to MR-CC hamper formulation of a theory applicable to general systems and extension to excited states [3].

Once spin-singlet and triplet pairs have been decoupled in double electronic excitation of CCSD referenced to the Slater determinant of the unrestricted Hartree-Fock (UHF) method, the stability and symmetry dilemma is solved and the modified CCSD method correctly behaves with respect to bond dissociation and transition states. The CCSD-level accuracy is recovered by recoupling double excitations of both the spin multiplicity. This modified CCSD theory named FSigCCSD implicitly describes static correlation related to the spin-triplet instability of the restricted Hartree-Fock (RHF) method employing the algorithms developed for the conventional CCSD theory [4].

This time, we have extended the FSigCCSD theory to excited states in the equation-of-motion scheme. The present work is a step towards a dynamics simulation method applicable to general chemical processes.

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Accelerated Hartree-Fock approach via reduced virtual orbital space

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We have shown an alternative way to obtain the Slater determinant ground state solution within an independent-particle approximation using the exponential ansatz for the wave function (Thouless theorem)[1] and exact treatment in terms of variational coupled cluster singles(VCCS) [2,3]. The non-terminating expansions of the wave function within the VCCS can be exactly treated by summing up the one-particle density matrix elements in the occupied block using simple recurrence relation. At the same time, this leads to an extremely simple diagonalization-free algorithm for the solution of the Hartree-Fock equations.
We apply this approach with a starting determinant using localized orbitals, i.e. we present a localized Hartree-Fock method[4]. The initial guess was obtained from diagonalising the Fock matrix constructed from the superposition of atomic densities. Starting molecular orbitals were localized using Pipek-Mezey procedure, or incomplete Cholesky decomposition of density matrix. Next, we were running VCCS iterations in local molecular orbitals. Convergence behavior and number of nonzero elements of T_1 amplitudes and density matrix were examined for series of medium sized molecules.
Furthermore we present unique algorithm[5] which reducing the virtual orbital space in VCCS approach and it significantly speed up the calculations.

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Low-cost Relativistic Coupled Cluster Method Based on Frozen Natural Spinors

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Relativistic effects play a critical role in accurately describing the electronic structure of heavy element systems. However, high-level relativistic methods, such as four-component coupled cluster (CC) theory, are computationally demanding, limiting their application to small systems. In this work, we present a low-cost yet accurate relativistic CC approach leveraging frozen natural spinors (FNS) derived from lower-cost correlated calculations. Natural spinors give a compact description of the virtual space and allow truncating a large part of the virtual space with little loss of accuracy[1]. Further simplification can be obtained by using a two-component atomic mean-field Hamiltonian (X2CAMF) and Cholesky decomposition of the two-electron integrals[2]. The standard FNS obtained from MP2 calculation does not perform very well for excited-states[3] and property calculations[4]. Special modifications to the FNS generation framework are needed to make it work beyond ground-state energy calculations. The FNS approach provides a practical route for extending high-accuracy relativistic quantum chemical methods to larger systems of chemical and technological interest, without compromising essential relativistic and correlation effects.

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Multireference coupled cluster method for the description of the dissociation of a single bond: the easy way

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This presentation is focused on the new quantum chemical methods enabling correct description of single bond breaking in ground and excited states for selected classes of molecules. The main reason for the difficulties in correct description of homolytic dissociation of a single bond using standard methods is that the closed-shell AB molecule dissociates into open-shell fragments, which makes it impossible to conduct correlation calculations based on a reference state based on a favorable Hartree-Fock function with spin restrictions. The solution to this problem, e.g. for diatomic alkali metal molecules, is to assume that the reference system is a two-positive ion with a closed shell, dissociating into closed-shell cations. Such a computational model makes sense provided that at the stage of correlation calculations we have a method that correctly describes the electronic states created after adding two electrons to the reference system, i.e. the electronic states of the neutral molecule. Such computational schemes, dedicated to determining double electron affinity (DEA), as well as triple electron affinity (TEA), are offered by the coupled cluster (CC) method within the multireference (MR) formulation [1] in the Fock space. The DEA-MRCC and TEA-MRCC methods were used in the calculations, which enabled the determination of precise energies of several dozen electronic states for points in the entire range of interatomic distances using a strictly size extensive method, and thus obtaining correct potential energy curves and the resulting spectroscopic properties for a number of diatomic compounds of alkali metals and alkaline earths. The obtained precise interatomic potentials can be useful for designing the syntheses of ultracold molecules. The applications of these studies are enormous, not only in chemistry but primarily in physics, e.g. in high-precision spectroscopic measurements.

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Ab initio calculation of magnetic Feshbach resonances in ultracold collisions between Rb (^{2}S) and AlF($^1\Sigma^+$)

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Recent advances in experimental techniques for generating and trapping cold and ultracold atoms and molecules [1] have brought attention to the importance of reliable theoretical predictions of ultracold collisions and reactions based on state-of-the-art *ab initio* calculations. In particular, the accurate calculation of magnetic Feshbach resonances is highly desirable, as these resonances play crucial roles in controlling collision outcomes [1, 2]. However, *ab initio* prediction of individual resonances remains a significant challenge.

In this study, we carry out scattering calculations to address the magnetic Feshbach resonances for the ultracold collisions between Rb(^{2}S) and AlF($^1\Sigma^+$), efficiently constructing the coupled-channel equations [3]. The interaction potential between Rb and AlF, as well as the geometry-dependent hyperfine coupling parameters (Fig. 1) are obtained with CCSD(T) and CCSD methods, respectively.

We found that the geometry dependence of the hyperfine coupling parameters in the short-range region of the collision complex is essential for the occurrence of Feshbach resonances. On the other hand, the resonance positions are primarily determined by the coupling between different rotational states, which is induced by the strong anisotropy of the short-range interaction potential.

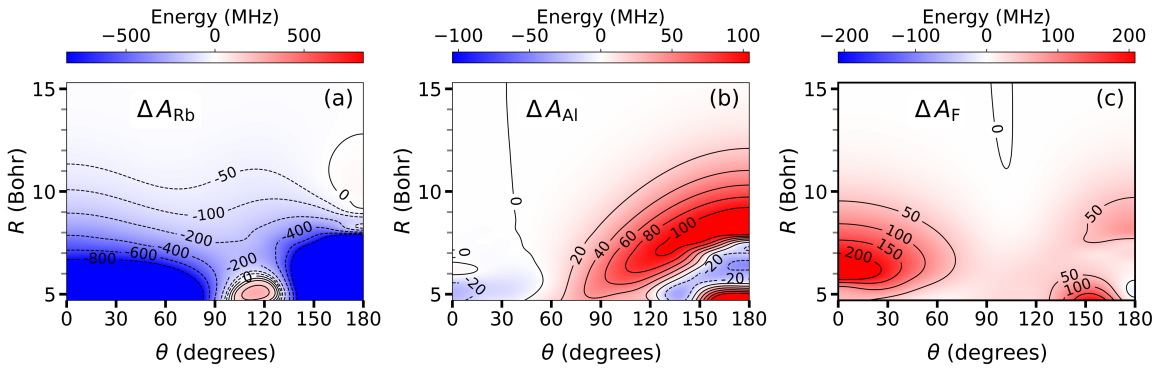

Figure 1: Hyperfine coupling parameters of the RbAlF complex. R denotes the distance between Rb and the center of mass of AlF (CM_{AlF}). θ is the angle of Rb-CM_{AlF}-F.

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pCCD-based computational strategies for large-scale modeling of organic electronics in the PyBEST software package

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The efficiency of organic solar cells (OSCs), typically composed of conjugated polymers as donors and fullerene derivatives as acceptors, is strongly related to their structure-property relationship. Example factors that play an essential role in the design of more efficient OSCs are the conformation of frontier molecular orbitals, the offset between the donor's highest occupied molecular orbital and the acceptor's lowest unoccupied molecular orbital, characteristic features of low-lying electronic transitions, and dipole moments. Unfortunately, OSCs' molecular size and their building blocks prohibit us from employing the most accurate state-of-the-art quantum chemistry methods. I will address this challenge with the pair coupled-cluster doubles (pCCD)-based methods and their extensions. [1, 2] Specifically, I will focus on (a) orbital energies [3], (b) dipole moments and quadrupole moments [4], (c) transition dipole moments [5], (d) embedding approaches[6], and (e) model Hamiltonians. Finally, I will demonstrate how these computations can easily be accelerated on hybrid GPU architectures like GH200.

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Neural network based algorithms for diabatization of electronic bases

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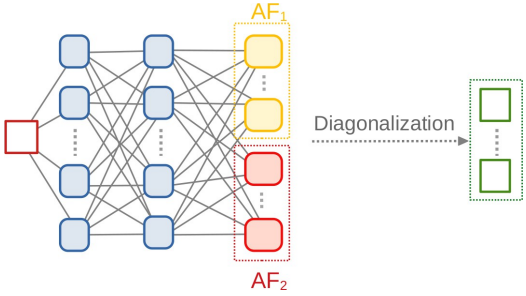
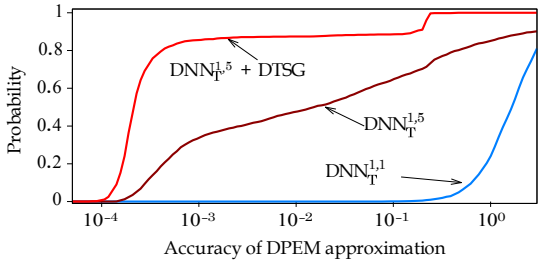
This work is motivated by the mathematical modeling of non-adiabatic processes of microscopic systems. At the core of this task we are concerned with finding a solution to the time-dependent Schrödinger equation. Using the well-known Born-Oppenheimer separation, this problem can be converted into a system of PDEs describing the motion of the nuclei of atoms. The form of this system is determined by the choice of the electronic basis, which is used to "discretize" the equation with respect to the electronic space variables. By choosing a special, so-called diabatic basis, we are able to cancel out some of the terms of this system that often cause bad numerical behavior. Finding the diabatic potential energy matrix (DPEM) is, however, a complicated task, since it is usually based on a detailed knowledge of different physical properties of the considered system.

In this work, we study an alternative diabatization approach based on the use of neural networks (DNN), which was firstly introduced in [*J. Chem. Theory Comput.* 2020, 16, 6456-6464]. It is designed to find a correct diabatic representation based on a very limited amount of training data - it needs almost exclusively adiabatic energies. Although the method looks promising, it is clear that under these assumptions, the task of finding the DPEM is fundamentally under-determined, which raises doubts about its reliability. Our goal is therefore to carry out a systematic investigation of the performance of the DNN method on several simplified one-dimensional models. To compare individual results, we present several statistical quantities illustrating not only the efficiency of the DNN method and limitations of its reliability, but also its sensitiv- ity to various internal parameters. Specifically, we study the effect of the choice of activation functions, different settings of the loss function parameters, or the number of hidden layers and neurons, and present several modifications of the original method that improve its behavior.





Acknowledgements: Work was partially supported by Grant of SGS No. SP2025/049, VŠB - Technical University of Ostrava, and grant no. VSB/24/021023. The calculations have been performed using the resources of the *IT4Innovations National Supercomputing Center of the Czech Republic* made available to us via grants no. OPEN-30-10, OPEN-32-47 and FTA-24-7. M. Ć . acknowledges support from the *Barrande Fellowship Programme for Cotutelle*.

Quantum-mechanical calculations of large molecular systems and analyses of interactions

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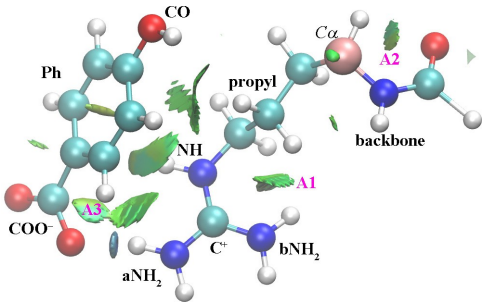
The cost of quantum-mechanical (QM) calculations can be reduced via fragmentation. There are many fragment-based methods. In this work, the fragment molecular orbital (FMO) method is used [1]. A protein can be divided into amino acid residue fragments. Then, fragments are computed in a polarizable embedding potential determined from the electron densities of all fragments. Interactions between fragments are computed by performing QM calculations of pairs of fragments in the embedding potential. The total energy for a system divided into N fragments is obtained as the sum of polarized fragment energies E_I' and interactions ΔE_{IJ},

$$E = \sum_{I=1}^{N} E_I' + \sum_{I>J}^{N} \Delta E_{IJ} \qquad (1)$$

Using analytic gradient of E, one can perform **geometry optimizations** and **MD** simulations of systems containing hundreds or thousands of atoms [1].

Pair interaction energies ΔE_{IJ} provide important information on the hotspots, for example, on residues J in a protein that bind a ligand I. FMO can be used in the partition analysis (PA) [2], in which it is possible to define interaction energies ΔE_{ij} for arbitrarily small molecular units called segments, denoted by i and j, for example, functional groups in a ligand and residues, so that a **rational drug discovery** process can be guided by simulations.

A graphical representation is obtained with the non-covalent interaction (NCI) index [3], Fig. 1. FMO calculations can be performed using feely available GAMESS package.



i (ligand)	j (Arg-16)	ΔE_{ij}
Ph	Propyl	-1.4
Ph	C^+	-1.7
Ph	NH	-3.2
Ph	aNH_2	-1.7
COO^-	C^+	-6.3
COO^-	aNH_2	-11.7

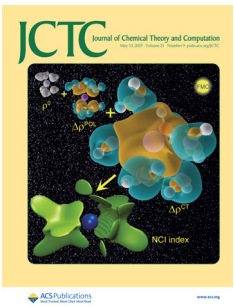


Fig. 1. Interactions ΔE_{ij} (kcal/mol) in Trp-cage protein (1L2Y) between functional groups in Arg-16 and ligand, visualized using NCI index (DFTB/PCM) [3], featured on the JCTC cover.

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Identifying residue relevance in biomolecular interfaces – beyond reading the tea leaves

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Molecular recognition and the formation of biomolecular complexes often involves contacts of large molecular surfaces. The rationalisation of these processes and the desire to understand the role of individual residues therein was for a long time based on to-some-degree reductionist views in both experimental and theoretical approaches. Personal experience, skill, and intuition of the researcher was usually instrumental in successful identification of such key residues. This, combined with the complexity of the myriad of residue interactions allowed the study of (bio)molecular interfaces on expert-curated datasets of limited size and diverse origins. With the advance of machine learning into the realm of chemistry and molecular biology, a necessity for a standardised, reproducible and quantitative method to rank the importance of residues in interfaces remained to be desired. We propose a new metric to address this problem – the singular value centrality CSV. It is based on a network model of the residue interaction topology [1, 2]. Submatrices of the weighted global adjacency matrix corresponding to interactions of subunits (e.g. proteins or domains) are subjected to SVD decomposition. The residue ranking is achieved by a reorganisation of the components in the resulting singular vectors. Herein, we lay the theoretical basis of CSV, demonstrate its' performance on a set of well known systems and discuss its' implementation in ready-to-use free open access code [3]. We propose a way to identify and threat water-mediated contacts and discuss some shortcomings of this method as well. Briefly, the extension to dynamic systems will be touched.

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Advancing the Buffer Region Neural Network Embedding Scheme (BuRNN) for Complex Molecular Environments

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The Buffer Region Neural Network Scheme (BuRNN) [1,2] addresses QM/MM boundary challenges by combining quantum mechanical accuracy with machine learning speedup. While BuRNN has been demonstrated for simple solutes in water, its applicability to larger, chemically diverse, and biologically relevant systems remains unexplored. Here, we present preliminary results applying BuRNN using Schnetpack [3] to more complex systems, such as benzene, and aspirin in water and Ca^{2+} in the active site of phospholipase. Our goal is to test the transferability of BuRNN to ligands with tens of atoms in realistic solvent mixtures and protein environments. Reference data were generated via classical MD, conformational sampling using the rigid-rotor harmonic oscillator approximation, and refined by active learning. Initial results show that BuRNN predicts energies and forces with accuracy comparable to the parent QM method. It also produces MD trajectories that match experimental structures and dynamics more closely than MM, while achieving an approximately 100-fold speedup compared to direct QM calculations. Ongoing work focuses on best practices for dataset generation and improving transferability across chemically related systems. Our ultimate aim is a general BuRNN model capable of reliably describing ligand–environment interactions in biochemical systems.

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Spin Frustration in Triangular Fe(III) MOFs: A Hidden Key to Reactivity

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High-spin (HS) DFT is widely used as the standard computational approach for modeling MIL-101(Fe) and related iron-based MOFs. However, our study reveals that this convention overlooks a critical electronic feature: spin frustration within the Fe_3O nodes. Using spin-flip DFT, we show that MIL-101(Fe) exhibits a spin-frustrated ground state, which the HS approximation fails to capture—leading to structural distortions, incorrect energetics, and misleading predictions of stability and reactivity. By explicitly accounting for spin frustration, we not only recover the correct structure but also provide a unified explanation for the framework's temperature-dependent N_2 and CO fixation behavior. At room temperature, spin frustration enhances N_2 binding, while upon heating its N_2 fixation activity is reduced but facilitates CO adsorption via π-back bonding.[1] These findings challenge the prevailing modeling paradigm and estab- lish spin frustration as an electronic feature that must be considered for accurate description of triangular Fe-MOFs.

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Small dots, Big effects: How size and functional groups affect the electronic and optical properties of MXene Quantum Dots

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The quantum confinement effect present in quantum dots (QDs) can significantly enhance properties such as chemical stability and electronic behavior compared to their two-dimensional (2D) counterparts. Among promising nanostructured systems, MXene-derived quantum dots (MXQDs) offer wide tunability through structural and chemical modifications. Despite increasing research interest, a comprehensive understanding of how different structural motifs and surface functional groups affect their electronic properties remains incomplete. [1]
In this study, we present a systematic theoretical comparison of various types of titanium-based MXene quantum dots (Ti_2CT_x) with different lateral sizes and surface functionalizations (T = –O, –F, –OH). We found that the band gap decreases with increasing size, and it becomes evident that it can be further tuned through appropriate surface functionalization, revealing opportunities for targeted engineering of electronic properties. [2] Additionally, we investigate their optical behavior, where time-dependent density functional theory calculations demonstrate that a change in surface functionalization induces a significant red shift in the absorption spectra. This study provides a perspective on the relationship between size, chemical composition, and the physical properties of MXQDs and outlines pathways for their application in nanoelectronic and optoelectronic devices.

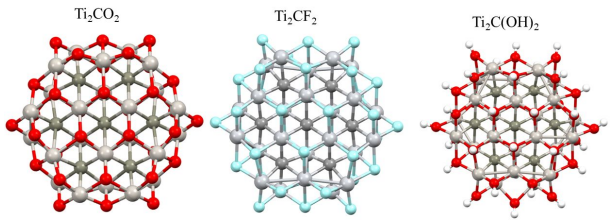

Figure 1: Optimized structure of fully saturated MXQDs with different functionalization.

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A density-based energy decomposition scheme for interacting fragments in periodic models and its insights into bonding and descriptors

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Energy decomposition analysis (EDA) schemes are a class of computational schemes that partition an interaction energy into several energetic contributions. To achieve that they employ the usage of constraints that are gradually relaxed in later steps. A rich class of them exist that differ primarily by those constraints, with the majority based on orbitals and applied in only molecular systems.

Here we discuss a density-based EDA scheme for partitioning interaction energies computed in periodic chemical systems and show the examples of its usage for both periodic and molecular systems. The method has a strong relation to a previously proposed density-based EDA (DEDA),[1] while taking additional advantage of the plane-wave regime in which the projector augmented wave (PAW) approach[2] is being used to computationally capture the behaviour of electron orbitals near the atomic nuclei. Like DEDA, our scheme functions by generating a "promolecule" in which valence electron density is equivalent to the superposition of the underlying fragments' valence electron density. Although schemes like this classically include terms accounting for electrostatic interactions, Pauli repulsion, effects of polarization and charge transfer within and between fragments, this scheme contains a different breakdown of the interaction energy that focuses more on electron density smoothly shifting through and/or near the fragment boundaries between steps.

The main advantages of our EDA scheme include its simplicity and also, importantly, allowing for the construction and visualization of two-state "Δ-functions" not only from the electron density (ie. Δρ's) but also from other differential functions of electrostatic potential [3,4] and the electron localization function (ELF). Overall it complements well other EDA schemes especially when used to compare two or more chemically related systems.

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Poster Abstracts

Hydroxyl radical initiated oxidation of methylmercury hydroxide in the aqueous phase: A theoretical study

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Methylmercury ($MeHg^+$), a highly neurotoxic organomercurial pollutant, poses significant environmental concerns, due to its environmental persistence, and bioaccumulation in aquatic food webs [1]. Methylmercury hydroxide (MeHgOH), a water-soluble mercury species, serves as a model compound for studying the environmental fate of methylmercury in freshwater and marine systems [2].

This work investigates the reactivity of methylmercury hydroxide (MeHgOH) with hydroxyl radicals ($^{\bullet}OH$) in the aqueous phase. Geometry optimizations were performed using Density functional theory (DFT) at the M06-2X/cc-pVTZ-PP level of theory. Single-point energy calculations were carried out using the single-reference coupled cluster method [CCSD(T)] with aug-cc-pVDZ-PP and aug-cc-pVTZ-PP basis sets, extrapolated to the complete basis set limit [CCSD(T)/CBS (aDT)]. Multiple reaction pathways were explored, including hydrogen abstraction (H-Abs), methyl abstraction (CH_3-Abs), hydroxyl abstraction (OH-Abs), and single electron transfer (SET). At 298 K, the energy profile indicated that the H- and CH_3-abstraction reactions exhibit the lowest Gibbs free energies of activation and are highly exothermic. The overall rate constant in water at 298.15 K was calculated as 1.99×10^7 M^{-1} s^{-1}. Among the competing channels, H-Abs from the methyl group, particularly H2-Abs and H4-Abs, were dominant, with a rate constant of 7.03×10^6 M^{-1} s^{-1}, contributing 35% of the total branching ratio (Γ). Kinetic analysis revealed that reaction rates increase across temperature range of 200 and 350 K. The lifetime of MeHgOH in the presence of hydroxyl radical at 298 K was predicted based on $^{\bullet}OH$ concentrations (10^{-18} M to 10^{-15} M) in natural water.

This work was supported by the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09I03-03-V05-0001 and the grant VEGA 1/0254/24 from the Ministry of Education Research, Development and Youth of the Slovak Republic.

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Progress in Generating Accurate Atomic and Molecular Gaussian Rydberg Basis Sets

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Despite the great success of quantum chemistry in the *ab initio* description of molecular ground and valence excited states, the treatment of systems strongly affected by Rydberg states or otherwise possessing extremely diffuse electronic character have been practically avoided in the *ab initio* quantum chemical studies in the past. The reason was the lack of suitable basis sets that could reach tens or even thousands of Å away from the molecular center, while at the same time remaining moderate in size. Moreover, the predominantly used Gaussian basis functions were considered inappropriate for the description of the diffuse states due to their rapidly decaying character.

In our recent study of lithium Rydberg states [1] we demonstrated that a systematically constructed tailored contracted Gaussian basis can easily reach tens of thousands Å (*i. e.* micrometers) from the origin with clear nodal structure while also offering unprecedented accuracy of the excitation energy, differing from the state-of-the-art explicitly correlated Gaussian approach only in the order of milihartree at the EOM-CCSD level. The developed method can also compute many more excited states than competitive approaches.

Further research [2] focused on eliminating the number of Gaussian primitives necessary for the construction of the contracted basis, allowing the use of standard quantum chemistry codes, and on refining the methodology so that the tailored Rydberg basis sets could be optimized routinely. A considerably more complex methodology for obtaining molecular Rydberg basis sets is still under development.

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Reorganization energies of extended organic oligomers from DFT perspective

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Reorganization energy defined as an energy that is released after an electronic transition (or ionization) in the process of geometry relaxation to the optimum structure for the final electronic state). The reorganization energies are important for spectroscopic studies, as they determine the fine structure and/or the band shape that is experimentally observed. They also play the key role in charge and energy transfer in the molecular crystals, thin films and organic polymers. They are, however, quite difficult to estimate from experimental data. Therefore it is essential to be able to obtain them independently, preferably from quantum-chemistry calculations.

The performance of the ab initio methods of obtaining the reorganization energies for important electronic transition in a series of unsaturated oligomers and their evolution with increasing chain lengths have already been assessed [1]. High cost of the correlated ab initio calculations, however, hinders their use for larger systems, which are often of interest for e.g. organic electronics. This calls for an analogous study that concern DFT methods. In this work we test the performance of several exchange-correlation functionals in calculating the reorganization energies for selected oligomers of thiophene and furan, containing up to 40 rings in the oligomer chain. Electronic transitions between the ground state, the lowest singlet and triplet states, and the anions and cations are studied. The excited states are obtained by means of the time-dependent DFT or, alternatively, using ROKS (S1) and ΔSCF (T1) methods, and the outcomes are compared in terms of the reorganization energy values and their evolution with the increasing chain length.

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A Generalized Framework for Excited-State Coupling in Molecular Fragments based on Second Quantization

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Second quantization (SQ) is a powerful framework for many electron systems. It is constructed to include the exchange interaction and can be applied for an arbitrary number of electrons. We aim to exploit these attributes and derive expressions for the coupling of non-covalently interacting chromophores.

The total Hamiltonian is partitioned into contributions from each monomer and their mutual interaction. The system's wavefunction is approximated as a product of the monomer wavefunctions, but due to their spatial overlap, this leads to complications in evaluating interaction terms using SQ.

To address this, a transformation of the annihilation operators is introduced using the inverse of the orbital overlap matrix,

$$\tilde{i}^- = \sum_p (S^{-1})_{ip} p^-. \tag{1}$$

This redefinition restores the desired anti-commutation relations and simplifies the calculation of matrix elements.

Excited states are constructed from local excitations on a monomer or as charge transfer states between them. These basis functions include both leading terms and corrections scaled by interfragment overlap, helping to distinguish dominant coupling contributions. Importantly, contractions between operators on different fragments vanish, streamlining the analysis. This is illustrated in an example, which provides insight into the importance and behaviour of charge transfer excitations throughout a potential energy curve.

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Tailored EOM-CC Methods for Electron Attachment Energies

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Accurate prediction of electron attachment (EA) and ionization energies is vital for modeling charge-transfer processes and electronic excitations in functional molecules. In this work, we present a comprehensive benchmark of Equation-of-Motion Coupled Cluster (EOM-CC) approaches based on frozen-pair reference states (EA-EOM-fpCC). These methods, built upon the pair Coupled Cluster Doubles (pCCD) ansatz and its orbital-optimized variant, which provide an efficient and cheap computational platform to model strongly-correlated systems.

A dataset of 24 organic molecules was used to evaluate several EOM-CC methods (fpCCD, fpCCSD, fpLCCD, fpLCCSD, CCD, CCSD) using the cc-pVDZ, aug-cc-pVDZ, and cc-pVTZ basis sets. In addition to direct EA predictions, we assessed the performance of energy difference calculations from IP-EOM and DIP-EOM states. All methods exhibited systematic convergence and were further improved via CBS extrapolation using a two-point fitting scheme. Our analysis revealed that fpCC approaches reach chemical accuracy comparable to CCSD(T), and leverage the poor performance of EA-EOM-pCCD in predicting EAs.

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Molecular Dynamics Investigation of Flavonoid–HSA Interactions

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Flavonoids (FL) are low-molecular-weight phenolic compounds known for their wide-ranging health benefits, including anti-inflammatory, anti-cancer, and neuroprotective effects. Despite their therapeutic potential, their clinical efficacy is limited by poor water solubility and low bioavailability [1]. Human serum albumin (HSA), the most abundant carrier protein in the bloodstream, plays a key role in enhancing the solubility, stability, and transport of flavonoids to target tissues. Binding to HSA not only prolongs flavonoid half-life but also modulates their pharmacokinetics through non-covalent interactions [2]. This study investigates the interaction of HSA with baicalein and scutellarein, using various computational and spectroscopic methods to evaluate their binding affinity and potential for therapeutic application.

Semi-flexible molecular docking was carried out using AutoDock 4.2.6 [3], with ligand geometries optimized at B3LYP-GD3/6-311G** level of theory and assigned Mulliken partial charges. The docking simulations targeted binding sites I–III of the apo form of human serum albumin (HSA) (PDB ID: 1bm0 [4]). The top-ranked docking poses were advanced to all-atom molecular dynamics simulations performed in GROMACS 2023.2 [5], employing the AMBER03 force field [6]. The Molecular Mechanics Generalized Born Surface Area [7] was employed to quantify the binding affinities towards HSA. The resulting binding free energies were corrected for the thermodynamics stability of the complex and compared with experimental values derived from spectroscopic measurements for validation of the computational model.

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Transition metal complexes: closed shell state stability and DFT vs. CASSCF comparison

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Several transition metal complexes will be highlighted to consider the performance of DFT calculations compared to CASSCF/NEVPT2 ones. These will include two-center copper and chromium complexes, ketimides of the Ti-Co series, and selected carbazone complexes of copper [1-5], see Figure 1. We will show several examples where the restricted singlet Kohn-Sham state is found to be unstable, leading to a broken-symmetry unrestricted singlet state. We will consider the antiferromagnetic contribution within the singlet CASSCF wave function in selected cases. The ordering of the spin states and further details of the electronic structure will also be touched upon. Theoretical calculations were performed with Gaussian16 [5] and Orca4-6 [6-8] packages.

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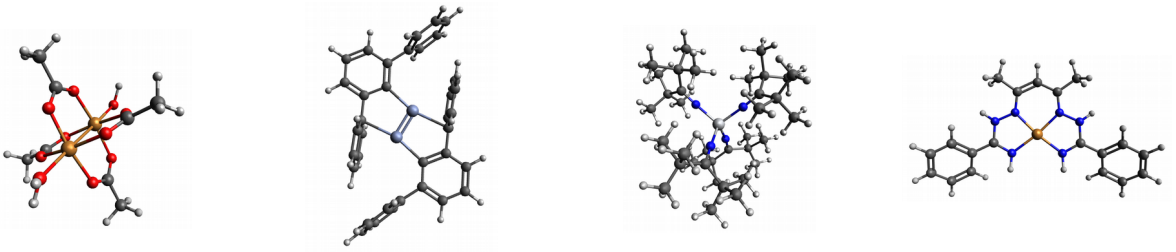

Figure 1. Two-center copper and chromium complexes, ketimides of the Ti-Co series, and selected carbazone complexes of copper

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Global Optimization of Cluster Structures via Genetic Algorithm

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This work presents a computational approach for determining the global energy minimum structures of clusters using genetic algorithms. The study first outlines the theoretical background of global optimization and genetic algorithms, then applies these concepts to the domain of cluster/aggregate optimization. The main outcome of this research is the development and implementation of a program, GenCluster, which employs a genetic algorithm to efficiently search for the lowest energy configurations of molecular aggregates. The design and implementation of this algorithm are described. Validation of GenCluster's performance is presented through a comparative study on small water and gold clusters, demonstrating its reliability and significant speed advantage over more systematic methods, albeit with a trade-off in exhaustiveness [1,2]. Finally, we present the successful application of this methodology to the aggregation of R123 dye.

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A Computational Study of NiO Polymorphism

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Nickel oxide (NiO) is a prototypical antiferromagnetic transition metal oxide widely employed as a benchmark system for investigating electronic correlations, magnetic exchange interactions, and oxide materials more broadly. To date, the only known phase of NiO with this stoichiometry adopts the NaCl-type structure, which has been experimentally observed in both bulk and nanoscale forms. Despite the fundamental significance of NiO, its potential polymorphism has not been comprehensively explored - likely due to the remarkable stability and broad applicability of the NaCl-type phase under ambient conditions. However, recent advancements in materials synthesis and characterization techniques have opened new avenues for discovering metastable or previously unrecognized polymorphs and properties - such as the high-pressure-induced metal-insulator transition in NiO [1]. Motivated by these developments, we present a systematic investigation of NiO polymorphism. Employing evolutionary algorithms combined with density functional theory calculations, we generate and fully optimize a diverse set of candidate crystal structures. From this dataset, we identify and assess possible polymorphs, analyzing their thermodynamic stability and magnetic configurations, including both high-spin and low-spin (experimentally unobserved) states. Our findings lay the groundwork for the potential synthesis of new NiO phases, further expanding the functional landscape of this versatile material.

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Molecular Properties with pCCD-based Methods

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The development of reliable and computationally inexpensive quantum chemistry methods for predicting molecular properties is still an active area of research. In this context, the pair coupled cluster doubles (pCCD) method has been developed and applied for a range of chemical problems, utilizing its ability to model strongly correlated systems. [1] Several strategies for dynamical correlation corrections, such as frozen pair CC (fpCC), [2] frozen pair linearized CC (fpLCC) [3], have been explored by our group to improve the performance of the pCCD method. Single-electron property estimations using these pCCD-based methods with both response and expectation-value approaches in the PyBEST software package have been recently implemented by us. [4] The main advantage of the expectation-value approach is that, unlike the response approach, there are no additional Λ-equations to be solved. In this work, the performance of pCCD-based methods in terms of dipole and quadrupole moments has been investigated using both response and expectation-value approaches. Electric multipole moments and dipole moment surfaces of a molecule contain crucial information about its electronic structure and spectroscopic properties. Dipole moment surfaces of a typical example, the HF molecule, are also created using these methods to investigate the performance of pCCD-based methods beyond the equilibrium regime. Our work indicates the importance of orbital optimization in the pCCD model and highlights the limitations of linearized CC corrections in predicting multipole moments. [5] The performance of the fpCCSD model, on the other hand, is found to be very close to CCSD, in the expectation value CC framework. [6]

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Integral Package for More Flexible Quantum Chemical Simulations

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We present a first version of *libani* [1] integral library for analytical anisotropic Gaussian (aniGTO) integrals evaluation for quantum chemistry software. The aniGTO basis set refers to a type of Gaussian basis function where the exponents can differ along different spatial directions - i.e., they are direction-dependent (anisotropic)

$$\chi_{a,\xi}^{aniGTO}(r) = x^{a_x} y^{a_y} z^{a_z} \exp(-\xi_x x^2 - \xi_y y^2 - \xi_z z^2)$$

where ξ_x are the exponents in $i = x, y, z$, accordingly. This feature allows aniGTOs to be elongated or compressed in specific directions, giving additional flexibility and adaptation to different physical regimes e.g.:

- quantum dot modeling
- molecular systems under anisotropic confinement
- faster convergence for systems with directional confinement
- magnetic field simulations
- reduced dimensionality problems (2D, 1D chemistry)

The library provides the Python API to evaluate one-electron / two-electron integrals for Cartesian aniGTO type functions, which can be easily interfaced with PySCF or PSI4 quantum chemical packages, enabling the use of any quantum chemistry method available within these software. As a proof of concept, we show the results of applications of aniGTO functions in non-symmetrical quantum dots, quasi-1D, and quasi-2D electronic structure modeling. We show that our results are consistent with previously published HF and FCI data reported in Ref. [2].

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No Heme-Chlorite Adduct in the Catalytic Cycle of Chlorite Dismutase: Insights From QM/MM and Dynamics Calculations

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Chlorite dismutase (Cld) is one of the rare enzymes capable of forming oxygen-oxygen bonds. Cld has been identified in a very small number of anaerobic bacteria that can use perchlorate as the final electron acceptor in their electron transport/respiration chain. It has been proposed that the catalytic cycle of Cld involves the binding of chlorite to the enzyme's active site, followed by the cleavage of one of the Cl-O bonds, leading to the formation of a high-valent iron-oxo center and a ClO radical/ion, and then a reorientation to the oxygen atom bound to iron, followed by the release of chloride and molecular oxygen. However, direct experimental confirmation of the existence of a chlorite-heme adduct in Cld is still unavailable, nor is it clear what the coordination mode of chlorite is. Moreover, reaction intermediates have not been directly observed in experiments. Previous DFT calculation from us and others have concluded that hemes cannot form stable adducts with chlorite – unlike, e.g., metallacorrins such as cobalamin [1]. This paper the results obtained from QM/MM optimization and QM/MM molecular dynamics calculations on the catalytic cycle, revealing compelling computational evidence that a chlorite-heme adduct in Cld is unlikely to be observable experimentally.

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Reducing Numerical Precision Requirements in Quantum Chemistry Calculations

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The growing demand for deep learning compute resources has led to the development of new kinds of low precision hardware. This talk explores how electronic structure calculation software can coexist on these AI-centric platforms. We will begin by examining in detail the numerical precision requirements of key computational kernels (including density functional theory and wavefunction methods). We will demonstrate that double precision often provides far more precision than is necessary. Then, we will present an approximation built from an error-free transformation of matrix multiplication that can exploit these relaxed requirements [1]. This approximation (called the Ozaki-scheme) will allow us to run calculations on high performance low precision hardware while obtaining the required precision (and no more) [2].

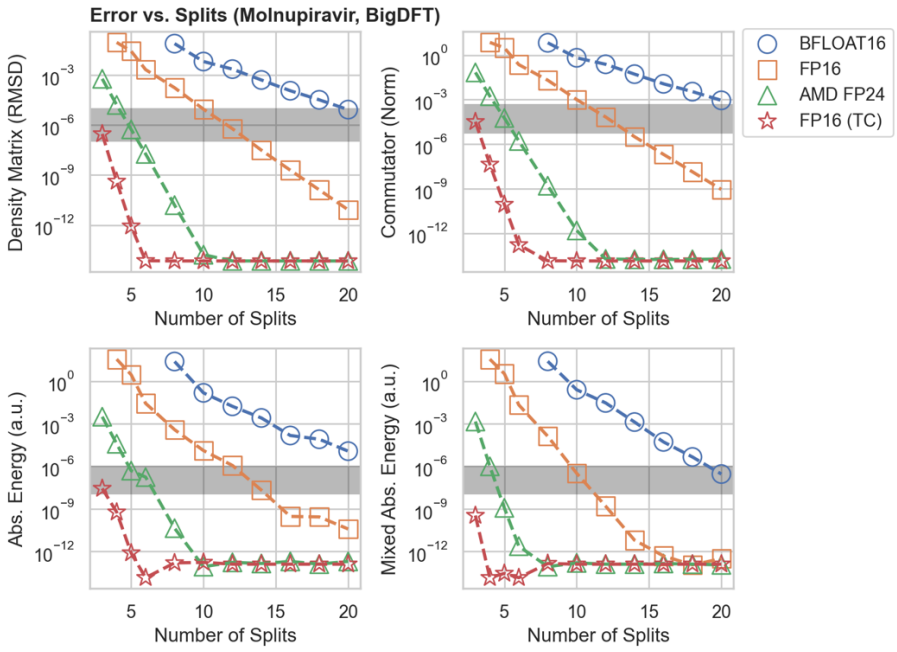

Figure 1: Convergence of errors when using the Ozaki-scheme with various low precision types and different numbers of splits. Errors below the gray bar are acceptable for production use.

Acknowledgements: Computations were performed using resources at the Research Center for Computational Science, Okazaki, Japan (Projects: 23-IMS-C029 and 24-IMS-C151).

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Tailored coupled cluster study of singlet-triplet gaps in cyclazine, heptazine, and cycloborane

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The excited states of organic chromophores and their energetics have been studied extensively over the years. Singlet triplet gap plays an important role for photophysical processes, where large gaps are typical for materials demonstrating singlet fission, while small gaps are connected with thermally activated delayed fluorescence. According to Hunds's rule, the first excited singlet state lies energetically above the the triplet state. However, there are exceptions to this rule. One such example of inverted singlet triplet gap are triazulenes [1, 2].

In this poster we present a study of inverted singlet triplet calculated by tailored coupled cluster method [3, 4] for three molecules: cyclazine, heptazine, and cycloborane. Two tailored space are employed: a smaller one consisting of the π orbitals on the aromatic rings, and a larger one selected based on orbital entropies. Results of these calculations confirm the inverted character of the singlet-triplet gap. Comparison with results of MkCCSD(T) method is also included.

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Exploring Intermolecular Interaction Through Variational Lens

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A key feature of Symmetry-Adapted Perturbation Theory (SAPT) [1] is the composition of interaction energy with physically significant terms such as: electrostatic, exchange, induction and dispersion. Among these, the induction energy plays a significant role, specially for strongly bonded systems. However, the induction terms in perturbation theory diverge and the low order terms do not recover the total induction. The missing higher order induction can be incorporated with $\delta_{\text{int}}^{\text{HF}}$ correction, resulting into a hybrid theory. While the $\delta_{\text{int}}^{\text{HF}}$ correction is important for H-bonded systems, but it is also known to overbind dispersion-dominated complexes. Therefore, it would be ideal to recover the induction effect in a consistent theory. One such approach is Pauli-Blockade (PB) [2] method, which offers a variational framework for infinite-order induction. However, because of the orthogonalisation step and subsequent loss of monomer identity, this theory is not useful for further SAPT-like development.

In this work, we explore intermolecular interactions through a variational approach termed as Symmetry-Adapted Relaxation Theory (SART), which is motivated by PB method but maintains monomer identity, therefore retaining SAPT-like character. Our methodology formulated in second quantization, is implemented using Psi4NumPy [3], a Python-based interface for the computational chemistry software Psi4. We report the agreement between interaction energy computed using our approach and supermolecular Hartree-Fock energy, demonstrating that variationally relaxed monomers effectively capture induction effects to infinite-order in the interaction operator.

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From Fermion Sign Structure to Static Correlation

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Static correlation, the failure of single-reference methods in complex fermionic systems, can be linked to topological differences of between mean-field and exact wavefunction sign structures. Contrasting variational minimizations under mean-field and exact nodal constraints decomposes the correlation energy into symmetric and antisymmetric components. The latter corresponding to a *nodal-penalty* term linked to Dirichlet *static* boundary conditions and fermion-sign problem. The technique provides precise partition of correlation energy, unifies orbital- and real-space perspectives on electron correlation and promotes diagnostics and trial wavefunctions that explicitly involve wave function nodes.

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Comprehensive Docking Prediction of Compounds Targeting the SARS-CoV-2 Main Protease

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The vastness and continual growth of chemical space make it increasingly difficult to efficiently identify potential drug candidates, even when advanced virtual screening methods such as molecular docking are employed. Our study therefore focuses on accelerating drug discovery by predicting and assessing the docking scores of hundreds of millions of compounds targeting the main protease of SARS-CoV-2, specifically its active site composed of the catalytic dyad, His41 and Cys145 [1]. The candidate molecules were sourced from the ZINC15 database [2], which organizes compounds into subgroups (A–K) based on criteria such as molecular weight and various physicochemical features. Due to the overwhelming number of structures, we employed a pre-screening approach using five machine learning models [3] built with the SchNetPack framework [4] to predict docking performance. Compounds with predicted scores below –11 kcal/mol were shortlisted and subjected to molecular docking using AutoDock Vina [5]. This allowed us to refine the predictions and assess the accuracy of the machine learning models.

Of more than 616 million compounds, 14,921 structures met the selection criterion based on predicted docking scores. Subsequent validation through molecular docking identified 10,202 of these structures as true positives, with docking scores lower than –11 kcal/mol. Precision, defined as the ratio of true positives to the total number of predicted positives (true positives plus false positives), ranged from 0.21 to 0.69 for the selected structures. Allowing a deviation of ±1 kcal/mol in docking scores increased the precision range to 0.63–0.91.

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Non-Bonded Interactions in Empirical Force Fields: Revisiting Parametrization in Classical Models

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Accurate force field modeling of biomolecules remains limited by inaccuracies in the description of non-bonded interactions in classical potentials. While bonded terms, mainly dihedral parameters, have undergone substantial refinement in recent years, non-bonded interactions continue to be a major source of error. Traditionally, the Lennard-Jones (LJ, 12-6) model has been blamed for overestimating short-range repulsion and yielding inaccurate interaction profiles. However, our results suggest that the primary issue lies in the parameter values themselves, not necessarily in the functional form of the potential.

By re-optimizing LJ parameters of small model molecules, we achieve significantly better agreement with DFT-derived reference data—even without modifying the underlying LJ potential—reinforcing the conclusion that parameterization, rather than potential form, is the dominant source of error. Furthermore, we show that the widely used Lorentz-Berthelot combination rules contribute notably to inaccuracies, particularly in polar/non-polar systems such as methane...water.

We further assessed the Exponential-6 (Exp-6) potential, using the approximation of Lim et al., as an alternative with less steep short- range repulsion. While Exp-6 improves short-range behavior in some cases, it does not consistently outperform the LJ model and, as expected, introduces higher computational cost.

These findings suggest that refining parameters within the standard LJ model may be a more practical and effective route to enhancing the physical realism of biomolecular force fields.

Spin-free SC-NEVPT2 Method for the Quantum Embedding of the Open-Shell Systems

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High-level electronic structure models are essential for the correct description of molecular systems. These methods, however, suffer from unfavorable scaling with respect to system size, which limits their applicability. On the other hand, in many cases, such as the molecular recognition problem and the exploration of the chemical reaction mechanisms, only a small region of the large system is important for the process of interest. In those cases, it is usually sufficient to apply the high-level model on the relevant fragment only, while the rest of the system can be described with the low-level mean-field approaches. Quantum embedding methods, such as projection-based embedding [1], density matrix embedding theory [2], and bootstrap embedding [3], exploit this principle and have been successfully used to model large scale systems.

Embedding methods can yield fragments with significant multiconfigurational character, for which adequate electronic structure models, such as active space approaches, must be used. Density matrix renormalization group (DMRG) with the N-electron valence state perturbation theory (NEVPT2) has emerged as a go-to method for these cases [4]. In the case of systems with local open-shell regions, embedding methods can yield different effective potentials for the embedded α and β electrons, which is incompatible with the spin-free implementations of NEVPT2. Spin-free variant, however, has a more favorable scaling with respect to the active space size. We therefore developed an extension of the spin-free strongly contracted NEVPT2 method that treats the spin-difference term as a perturbation and works out-of-the-box with the commonly used spin-free DMRG software [5]. We present the results obtained by applying this method to the selected systems of interest to demonstrate its efficiency and accuracy.

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Theoretical prediction of novel palladium oxide phases based on ion beam synthesis experimental data

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Palladium and its compounds are essential in various industrial fields, such as automotive, pharmaceutical, and agriculture - mainly due to their catalytic properties. Recently, palladium oxides have also gained attention for their potential catalytic applications [1], although only two forms, PdO [2] and PdO_2 [3] are currently well-characterized. In this study, we aim to predict the crystal structures of previously unreported palladium oxide compounds: Pd_2O, Pd_3O_4, Pd_4O_5, and Pd_5O_4. Our investigation is driven by experimental results from reactive magnetron sputtering and ion implantation, which yielded X-ray diffraction (XRD) patterns. These findings suggest the formation of novel oxide structures with Pd:O ratios that deviate slightly from the conventional 1:1 stoichiometry. To explore and validate these potential new phases, we employ a hybrid computational approach combining Density Functional Theory (DFT) with Evolutionary Algorithms (EA).

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UV Chromophore Excited with Visible Light: CO Release from Flavonol

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Carbon monooxide (CO) is a toxic gas. However, when applied properly, it has been reported to provide anti-inflammatory effects with applications in transplant surgery, microbial infections, oncology, cardiovascular diseases etc. [1, 2]. Therefore, a whole family of the so-called CO--releasing molecules (CORMs) has emerged. Flavonol, being photoactivable CORM (photo-CORM), is known to release CO when brought into a triplet state [3]. However, its excitation to the S_1 state, what can be followed by an intersystem crossing (ISC) to a triplet state, requires an UV radiation which can damage human tissues. It was shown that when linked to a porphyrin molecule functioning as a visible-light absorbing antenna, flavonol can accept a triplet excitation via the so-called *proton-coupled triplet energy transfer* [4]. Thus, we can use safe visible light to excite the UV absorbing flavonol. In this work, we extend the story with phthalocyanine as the absorbing antenna. Our collaborators from Masaryk University observed that when irradiated with 610 nm light, a mixture of zinc-phthalocyanine and flavonol produces CO in reasonable quantum yields. We used tools of quantum chemistry to characterize and model the process of energy absorption by phthalocyanine followed by transfer to flavonol. Our investigation explores three scenarios: (I) ISC of phthalocyanine to a triplet state followed by a triplet energy transfer to flavonol, (II) direct energy transfer accompanied by ISC from the S_1 state of phthalocyanine to the T_1 state of flavonol, and (III) the role of an electron transfer between excited phthalocyanine and flavonol. The calculations involve an accurate DLPNO-CCSD(T) level of theory as well as dynamical studies to mimic the vibrational dependence of excitation energies.

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Relativistic iterative linear damped response TDDFT solver for predicting X-ray absorption spectra of open-shell molecules

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The damped response time-dependent DFT method (DR-TDDFT), or also known as the complex polarization propagator approach is a perturbational method used as an alternative to standard eigenvalue TDDFT. The method provides better applicability in systems with high density of states or in high-frequency domains. The size of the systems commonly computed are too large for direct calculations to be viable, which only leaves iterative approaches as a practical solution. The present iterative subspace solver considers hermicity and time reversal symmetry [1,2], and is applicable only to closed-shell singlet configuration systems. Methods for treatment of open-shell systems require the separation of time-symmetric general terms into symmetric and antisymmetric parts, which provides a new layer of complexity. The goal of this project is to extend the scope of the DR-TDDFT methodology by developing the formalism that allows the inclusion of open-shell systems, include it in the ReSpect software package, and assess the performance by comparing the results with experimental data.

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In silico modeling of reactions using machine-learned neural networks

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Accurate description of metalloenzymes remains challenging, due to the specific electronic properties of the transition metals. The coordination of ligands and the chemistry that takes place at the metal centers typically requires a quantum mechanical description of interactions, while standard molecular dynamics simulations are most efficiently performed with classical force fields. Hybrid quantum mechanics/molecular mechanics (QM/MM) simulations offer the possibility to include electronic degrees of freedom. In this project, we will approximate the metal-centered active site of metalloenzymes by Buffer Region Neural Network approach (BuRNN), which is a multiscale QM/MM approach, facilitated by machine-learned potentials. In short, the method introduces a buffer region, significantly reducing interfacial artifacts in common QM/MM approaches. The additional costs in terms of computing power are compensated by approximating the QM energies and forces with a machine-learned potential. In this particular case, the classical simulations are performed by the GROMOS software, while the QM interactions are learned using the SchNetPack tools. Two main challenges were identified to extend the BuRNN methodology to radical reactions in metalloenzymes.The neural network needs to be trained for reactivity, such that reactions can be monitored. While BuRNN had already been successfully applied to single metal ions in solution[1]. and to small organic molecules, reactions had not been described yet. Second, the complexity of the buffer and outer regions has to be increased, to entail not only simple solutions, but also an enzyme environment. For this, a sufficient amount of reference data is to be generated. In view of the developments in the field, we decided to slightly shift the intended timeline and focus on the first challenge. As a simple model system for chemical reactivity, we started with simulating chloromethane, and to subsequently describe a simple SN2 reaction.

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Improving docking score predictions through training dataset enrichment

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The search for computationally efficient methods for initial screening of candidate molecules in traditional in silico drug design workflows remains highly relevant, especially if these methods can achieve accuracy comparable to docking with significantly improved computational speed. In this study, we focus on enhancing the accuracy of docking score predictions for inhibitors targeting the SARS-CoV-2 main protease (Mpro). Docking scores were calculated using the AutoDock Vina 1.2.2 software with the standard AutoDock scoring function [1].

Based on our previous studies [2,3], which primarily focused on improving prediction accuracy through exploring various machine learning (ML) models and fine-tuning their parameters, the current investigation explores alternative strategies - specifically, enrichment of the training dataset. We systematically tested multiple enrichment approaches, which involved transferring selected compounds from a larger test set (~170,000 compounds) into the training set (~60,000 compounds), with the goal of significantly improving predictive performance on unseen molecules. The neural network model was constructed using the Keras/TensorFlow framework, and SOAP (Smooth Overlap of Atomic Positions) descriptors were used to represent molecular structures.

The central research question addressed is whether the predictive accuracy of existing ML models can be more efficiently enhanced by targeted enrichment of the training dataset, or if constructing entirely new ML models specifically tailored to each new dataset is necessary. Our findings provide insights into effective dataset enrichment strategies and practical recommendations for improving computational efficiency and predictive performance in virtual screening workflows.

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Investigating Excited-State Charge Transfer in Donor–Bridge–Acceptor Systems with EOM-PCCD+S

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We introduce a new domain-based charge-transfer analysis tool[1, 2], applied to the first excited state of several dye molecules proposed as prototypical sensitizers for dye-sensitized solar cells (DSSCs). Specifically, we focused on investigating the influence of lone pairs located in the bridge domain on the electronic properties of these dyes.

A unique feature of the proposed model is its ability to both quantify and trace the direction of charge flow between different molecular regions or moieties. This is achieved by analyzing the weights of the coefficients c_i contributed to excitations in the excited state calculated with EOM-pCCD+S[3] using optimized, naturally localized pCCD orbitals.

These excitation contributions were further classified according to the molecular domain (donor, bridge, or acceptor) and the excitation type (local vs. charge transfer). The resulting hole and particle character for each domain was then compared to the corresponding analysis based on the transition density matrix[4], obtained from TD-CAM-B3LYP.

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The effect of orbital optimization and correlation correction in spin-unrestricted geminal models

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The antisymmetrized product of strongly orthogonal geminals (APSG) Ansatz can be variationally improved through orbital optimization as well as by solving local two-electron Schrödinger equations, albeit at the expense of spin-symmetry breaking. This can be partially corrected using half-projection (HP). Distortion potential energy curves of HP-APSG are investigated for benzene using atom-centered, bond-centered, and delocalized orbitals, highlighting the role of parameters in the geminal coefficient matrix [1]. To account for dynamic correlation, two perturbative approaches are presented that can utilize HP-APSG as reference wave functions. A pivot-invariant, frame MCPT [2] based multireference extension of the perturbation-adapted (PAPT) method [3] is introduced and compared with the weak and strong symmetry-forcing schemes of the Dyall-type spin symmetry-adapted (SAPT) method [4, 5].

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DFT and CASSCF Cr^{I}–Cr^{I} bond characterization and what can do quantum crystallography

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The studied system (**S**, Figure 1) is based on the published complex [1] in which the Cr^{I}-Cr^{I} unit is stabilized by two monovalent terphenyl ligands Ar'CrCrAr' (Ar' = C_6H_2-2,6(C_6H_3-2,6-Pr^{i}_2)$_2$-4-$SiMe_3$). The structure can be found in the Cambridge Crystallographic Data Center (CCDC) under the code 681728 or the identifier SIYNAQ. The Cr^{I}-Cr^{I} bond of studied system was characterized using single-determinant DFT (BLYP, B3LYP, ωB97X-D and M06-2X) and multi-determinant CASSCF/NEVPT2 approaches. The focus was directed mainly on the similarities between bonding parameters of both methods but also on the energetics [2].

Further analysis involved studying the effects of spin state preference and methodology on structure factors magnitudes, which are essential to assess the electronic structure which is atomic density basis set Schrödinger dependent, but the final electronic structure is Schrödinger independent (a least squares fit of experimental a theoretical structure factors) [3].

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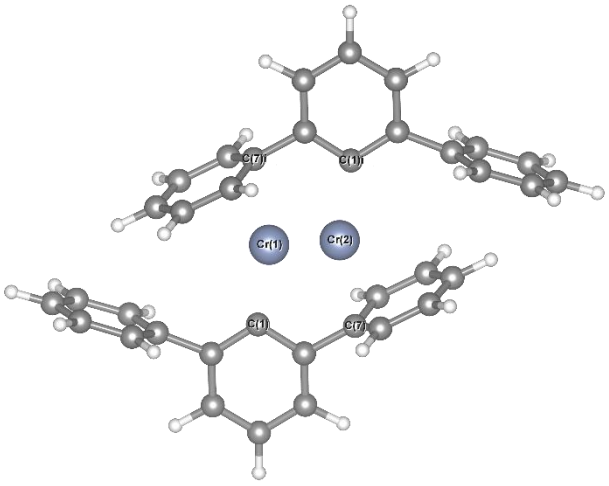

Figure 1. Complex **S** ($Ar^{S}CrCrAr^{S}$ (Ar^{S} = C_6H_3-2,6(C_6H_5)))

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Accurate nuclear magnetic dipole moments of ^{77}Se and ^{123,125}Te isotopes

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Accurate ab initio calculations combined with NMR experiments [1-2] offer a more reliable way to determine nuclear magnetic dipole moments, going beyond older approaches that rely on outdated diamagnetic corrections [3]. In this study, we present high-precision NMR shielding calculations for selenium and tellurium compounds. We replace traditional reference systems (SeO_3^{2-} and TeO_3^{2-}) with modern, well-defined NMR standards [4]: $Se(CH_3)_2$ and $Te(CH_3)_2$. We analyze the effects of basis set size, electron correlation, relativistic contributions, and solvent environment, and carefully estimate the uncertainties in our results. Using these improved standards, we re-evaluate the magnetic dipole moments of the ^{77}Se, ^{123}Te, and ^{125}Te nuclei, leading to updated recommended values. The calculated shielding constants establish accurate absolute shielding scales for selenium and tellurium. These revised nuclear moments provide valuable reference data for nuclear physics, especially for determining magnetic moments in isotopic series through hyperfine interaction measurements [5].

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Efficient Koopmans'-Based Orbital Energy Predictions for Organic Solar Cells Using pCCD type methods.

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This work introduces computationally efficient strategies to predict orbital energies in molecular systems, with a focus on organic solar cell (OSC) materials [1]. The methodology utilizes the pair Coupled Cluster Doubles (pCCD) framework and its orbital-optimized variant [2,3] to approximate ionization potentials (IPs), electron affinities (EAs), and the charge gap [4,5]. By integrating Koopmans-based methods into a canonical Hartree-Fock and embedding electron correlation effects through pCCD wave function and natural pCCD-optimized orbitals, we achieve accurate energy predictions at significantly reduced computational costs compared to conventional approaches.

Validation against theoretical and experimental datasets for atoms and 24 organic acceptor molecules confirms that Koopmans-based models employing pCCD natural orbitals deliver balanced representations of occupied and virtual orbitals. These findings underline the potential of geminal-based techniques, such as pCCD (implemented in the PyBEST software package) [6,7], as scalable and accurate alternatives to traditional wavefunction methods. This advancement bridges computational efficiency and predictive power for designing next-generation photovoltaic materials [8].

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The catalytic effect of copper complexes with non-innocent pentan-2,4-dione bis(amidrazones) ligand in CuAAC reaction. DFT study.

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The cycloaddition of azides and terminal alkynes using copper complexes (denoted as **4**) as catalysts (CuAAC) has been known since the beginning of the millennium [1-3]. However, to this day, there is no mechanism that can precisely describe it. A better understanding of the mechanism could facilitate the industrial-scale production of new materials and triazole-like compounds. This study provides a quantum chemical consideration utilizing the B3LYP/def2-TZVP computational protocol [4-6] together with the semi-empirical GFN2-xTB method [7,8]. Solvent effects for acetonitrile were approximated by the Integral Equation Formalism Polarizable Continuum Model (IEFPCM) [9,10] as implemented in Gaussian16 [4]. The reactants are benzyl azide (B) and phenyl acetylene (HA), respectively, and the product is simply HAB. We assume that the presence of A^- together with the formation of a **4**-A species is important for the reaction mechanism.

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Non-canonical α/γ backbone conformations in DNA and protein-DNA complexes

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The OL24 force field, developed at Palacký University, significantly advances molecular dynamics modeling of DNA by improving the stabilization of non-canonical backbone conformations and sugar puckers. Compared to its predecessor OL15[1], OL24[2] adopts the α/γ modification from OL21[3], increasing the population of α/γ = *trans* backbone states and introduces a modification that stabilizes the C3′-endo (northern) sugar pucker commonly found in A-DNA form near protein-DNA interfaces or ion/side-chain intercalation sites. By refining the deoxyribose dihedral potential and adopting the OL3[4, 5] glycosidic torsion (χ) parameters, OL24 yields a more balanced energy landscape between A- and B-DNA states, in better agreement with crystallographic and NMR reference data. OL24 outperforms OL15, OL21, and bsc1[6] in preserving native northern puckers and α/γ = *trans* conformers in simulations of protein–DNA complexes, while older force fields notably underestimate the stability of these conformers. These results underscore the critical role of force field choice for accurate modeling of biologically relevant DNA structural transitions during protein–DNA recognition.

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Relativistic DFT methods for predicting EPR parameters of species containing heavy elements

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In this work, we present a comprehensive solution for DFT calculations of the EPR g-tensor and hyperfine coupling tensor in heavy-element systems. Achieving accurate results requires: (a) a solid theoretical framework supporting DFT method development; (b) a state-of-the-art four-component (4c) methodology for benchmark values; and (c) a computationally efficient two-component (2c) approach that closely matches 4c results.

(a) Relativistic methods based on the Dirac–Coulomb–Breit (DCB) Hamiltonian set the standard in quantum chemistry. However, applying these methods to systems with nonzero spin and multi-determinant electronic states is challenging, as spin is not a good quantum number. Here, we review fundamental aspects of EPR theory and their validity within the DCB relativistic framework, addressing questions about the tensor nature, observability, and diagonalizability of the g-tensor, as well as the reliability of the standard EPR effective spin Hamiltonian and conditions for DFT predictions of EPR parameters. These and other aspects have been also discussed in refs [1,2] and works cited therein.

(b) The recently developed noncollinear Dirac-Kohn-Sham theory for calculating g-tensor [3]—based on the Dirac–Coulomb Hamiltonian, restricted magnetically balanced basis, and London atomic orbitals—enables practical computations and provides reference data for development of 2c methods.

(c) We present a computationally efficient atomic mean-field exact 2c method for prediction of EPR parameters [4]. The approach is for all practical purposes as accurate as the four-component methodology with a significantly reduced computational cost.

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Dressed pCCD: Efficient Modeling of Electron Correlation

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We present a custom implementation of the Dressed Restricted Pair Coupled Cluster Doubles (DR-pCCD)[1] method within the PyBEST framework, designed to improve the treatment of electron correlation in strongly correlated systems. DR-pCCD builds upon the pair Coupled Cluster Doubles (pCCD)[2,3] ansatz by incorporating effective triple and quadruple excitation contributions, $\hat{T}_3$ and $\hat{T}_4$, which are computed externally and used to dress the amplitude residual equations.

Our implementation integrates tightly with PyBEST's[4, 5] modular architecture, leveraging a symbolic contraction engine, and a flexible tensor reader that supports symmetry-aware parsing of spin-resolved amplitude data. The tensor infrastructure allows dynamic construction of dressed excitation spaces and efficient evaluation of residuals, facilitating black-box-like usage while maintaining high computational performance.

We validate our implementation using the 1-D Hubbard Hamiltonian, comparing energy and amplitude predictions against reference DMRG results. The DR-pCCD method improves upon pCCD while preserving computational simplicity and extensibility, making it a promising tool.

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On the keto-enol tautomerism of polycyclic aromatic hydrocarbons

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Large polycyclic aromatic hydrocarbons (PAHs) are significant environmental contaminants [1] that can be transformed into hydroxylated derivatives [2]. These hydroxylated PAHs exhibit keto-enol tautomerism, a chemical equilibrium involving an intramolecular proton transfer and a double bond rearrangement. The position of this equilibrium is highly sensitive to the molecule's structure, including the number and arrangement of its aromatic rings and the location of the hydroxyl group. Therefore, the primary aim of this work was to characterize this equilibrium by calculating the Gibbs free energies of tautomeric reactions for a series of PAHs containing up to five condensed benzene rings in an aqueous environment. Calculations were performed at the DFT level of theory using the Gaussian 16 program package [3], with solvent effects approximated by the implicit continuum model [4]. The resulting data yielded corrected $pK_T^{\sim}$ values (Fig. 1), which allowed us to predict the prevalent keto or enol tautomer for each compound studied [5].

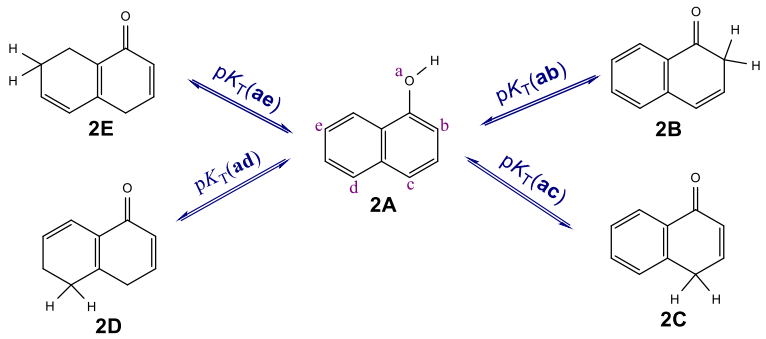

Fig. 1. Tautomers of naphthalen-1-ol under study and notation.

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Theoretical study on structure and interactions between cytomegalovirus glycoprotein UL141 and small glycomimetic antagonists

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Empirical (molecular docking) and quantum mechanics methods (QM/MM and QM FMO-PIEDA) were used to identify a binding site of iminosaccharide antagonists on a surface of glycoprotein UL141 of cytomegalovirus [1]. Three possible binding sites were predicted. The site near Trp235 and Asp232 of UL141 was predicted by FMO-PIEDA interaction energy calculations as the most likely. The theoretical prediction was further verified in experiments using mutational and binding analyses by SPR [1]. On the side of the antagonist, the major contributor to the interaction energy is the pyrrolidine fragment (84%–87%). The phenyl ring and short alkyl moiety presents only 9% to 14% and 2% to 4%, respectively. On the side of UL141, negatively charged amino acids Asp232, Glu164, Glu229, Glu230, and Asp228, which are in a direct contact with the antagonist, contribute most significantly to interaction energy. Few nonpolar amino acids as Leu163, Pro231, and Thr235 also contribute significantly.

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Mechanistic Study of the Conversion of Primary Alcohols and Butadiene to Branched Ketone Using Rhodium Catalyst

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The direct formation of ketones without premetalation is a major focus in catalysis research as it offers more straightforward reaction process and fewer steps [1]. Here we present our investigation of the mechanism for the conversion 3-methoxybenzyl alcohol and butadiene into branched isobutyl ketone with rhodium (I) complex catalyst under basic condition using density functional theory [2]. The reaction consists of four main steps: (i) oxidation of the alcohol reactant to generating the corresponding aldehyde and rhodium(I) hydride complex as active catalyst, (ii) hydrogenation of butadiene to form the allyl–Rh(I) complex, (iii) carbonyl addition from the allylic carbon to produce rhodium(I) alkoxide intermediate, and (iv) hydrogen transfer processes to generate the desired ketone product, which is released in its enolate form. The rate-determining states are in the carbonyl addition process (both intermediate and transition state) with an energy barrier of +30.4 kcal/mol. The formation of the linear ketone is hindered by steric effects from two PPh3 ligands bound to the Rh center throughout the reaction. Moreover, the positions of transferred hydrogens in our proposed catalytic cycle are consistent with the results of the deuterium labeling experiment, highlighting the hydrogen (auto)transfer process in this conversion of primary alcohol to branched ketones.

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Through-Space Spin-Spin Coupling Pathway Propagated via π-Orbitals

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Despite nuclear magnetic resonance (NMR) and in particular indirect nuclear spin-spin coupling (SSC) having gradually evolved into the most essential tool of chemical analytics, the interpretation of couplings between atomic nuclei separated by more than one single covalent bond has long suffered from a limited understanding of the propagation of said coupling through the molecular structure. The idea of coupling mechanisms that bypass covalent bonds altogether have come into focus of researchers[1]. However, studies of this so called "through-space" (TS) coupling have generally been limited to the propagation of SSC by atomic lone-pair orbitals. The role of π-orbitals in the propagation of SSC through a network of conjugated double bonds, has recently been explored by some of the authors[2,3]. Therein, the idea of a TS mechanism of SSC propagation via π-orbitals was not accounted for.
The current work uses theoretical tools to explore the possibility, abundance and significance of TS-SSC propagated by π-orbitals, not reported in the literature, nor utilised in contemporary analyses of NMR spectra.

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ML-based prediction of protein-ligand binding affinities utilizing atomic representations

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Accurately predicting binding energies between ligands and target proteins is critical in the early stages of drug discovery. In this work, we focus on inhibitors of the SARS-CoV-2 main protease (Mpro) and aim to train machine learning (ML) models as a computationally efficient alternative to molecular docking for affinity assessment.

State-of-the-art methods typically rely on sophisticated neural networks (NN), such as graph NN, convolutional NN or transformer architectures. In contrast, we investigate the potential of less complex, traditional ML approaches with substantially lower computational demands, such as Kernel Ridge Regression (KRR) and eXtreme Gradient Boosting (XGBoost). Unlike most NN-based approaches, which predict binding affinity by aggregating atomic contributions, traditional ML methods typically rely on molecular-level descriptors and predict only total binding affinity. Our main goal was to assess whether this difference in representation contributes to disparities in prediction accuracy.

While KRR can utilise either atomic- or molecular-level representations through the appropriate choice of similarity kernel, it only provides predictions for the total binding energy. To go one step further, we customised the loss function in XGBoost to both leverage atomic representations and predict atomic contributions to binding affinity directly. Preliminary results are promising, especially for larger and more potent compounds, though further evaluation is required.

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Voxel-based Computational Quantification of Rodent Brain MRI data

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Magnetic resonance imaging (MRI), combined with advanced computational tools, enables non-invasive investigation of structural brain changes in preclinical models. While primarily an imaging technique, its quantitative analysis relies on advanced computational and theoretical frameworks. In this study, we applied an optimized computational workflow based on established methods for brain MR image analysis, utilizing Advanced Normalization Tools (ANTs) [1], Convert3D (c3D), and MRtrix3 [2]. The workflow was adapted to our rodent maternal depression model dataset, acquired using a Varian horizontal bore MRI scanner.

The workflow includes MR image reorientation and spatial alignment to a virtual atlas coordinate framework. Preliminary manual alignment of the virtual Waxholm Space atlas to the T2-weighted MRI images was performed in ITK-SNAP [3], followed by automated rigid, affine, and non-linear registration using ANTs (antsRegistrationSyN.sh) [1]. ANTs was also used for transformation field generation. Anatomical structures were warped into subject-specific spaces using MRtrix3 for volumetric analysis, and brain region masks were transformed using the generated deformation fields [2]. The final step involved brain region-of-interest extraction from the virtual Waxholm Space rat brain atlas using c3D, followed by voxel-wise volumetric quantification of our masks through statistical evaluation of the masked regions by MRtrix3.

We found that this approach is suitable for the volumetric analysis of our rodent MRI data. Detailed volumetric quantification provides a foundation for correlating structural changes with neurotransmitter alterations, as well as for theoretical interpretations of brain function, particularly in various pathologies. However, further improvements and comparisons with other semi-automatic methods are needed to validate its accuracy and reliability.

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Transition metal clustering on carbon-based nanostructures and their hydrogen storage properties

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Graphene-based materials are nowadays extensively studied due to their potential utilization in many industrial applications. Electronic properties and reactivity of these materials can be significantly improved via modification with heteroatoms, such as transition metals [1]. The transition metal (hetero)atoms within these structures present reactive sites for example for H_2 attack [2]. Such interaction between the metal atoms and H_2 molecules can be utilized in hydrogen storage technologies. There are several distinct modes of metal-H_2 interaction, e.g. formation of η^2-H_2-bond (Kubas interaction) or H_2 activation leading to the dissociation of H_2 molecule. In one of our previous studies, we reported that planar graphene-based surfaces doped with single metal atom (Sc, Ti, V) can store up to 3 H_2 molecules via Kubas interactions [3]. It was also shown that the surface curvature can increase this hydrogen storage capacity up to 4 H_2 molecules per one metal atom [3]. In the presented study, formation of light transition metal (Sc, Ti, V) nanoclusters on finite size graphene-based nanostructures (C_{54} and C_{36}) is investiagted at the DFT level of theory. Additional insights into the nature of metal-H_2 interaction was provided by quantum theory of atoms and molecules. Our preliminary results suggest that C_{54} decorated with Sc_4 nanocluster (see Figure 1) can bind up to 9 H_2 molecules either via dissociation of H_2 molecules or by Kubas interactions. It is also found that the H_2 dissociation is energetically strongly favored over the formation of Kubas interaction.

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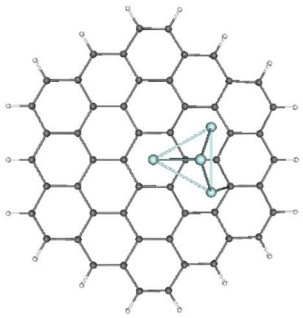

Fig. 1. Structure of C_{54} decorated with metal nanocluster Sc_4.

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A Descriptor Is All You Need: Accurate Machine Learning of Nonadiabatic Coupling Vectors

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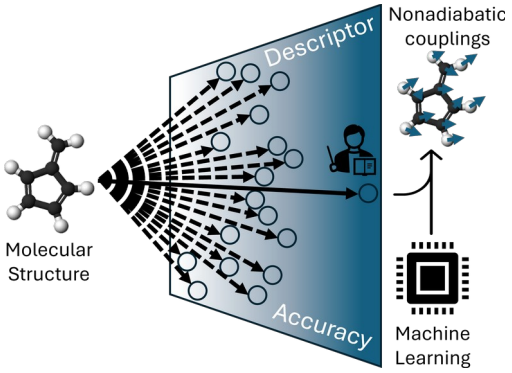
Nonadiabatic couplings (NACs) play a crucial role in modeling photochemical and photophysical processes with methods such as the widely used fewest-switches surface hopping (FSSH). There is therefore a strong incentive to machine learn (ML) NACs for accelerating simulations. However, this is challenging due to NACs' vectorial[1], double-valued character and the singularity near a conical intersection seam[2]. We combine multi-state ANI[3] model with kernel ridge regression for NACs, design NAC-specific descriptors and novel ML phase-correction procedure allowing learning NACs with accuracy of R^2 exceeding 0.99. This fully ML-driven FSSH dynamics leads to an accurate description of S_1 decay of prototypical fulvene targeting the SA-2-CASSCF(6,6) electronic structure level. Our implementations are available in open-source Mlatom.



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Stability indicators of hydrogenated Fullerenes

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Predicting stability of hydrogenated of fullerenes. The Isolated Pentagon rule successfully correlates with stable fullerenes, but fails to differentiate among stable isoforms; various graph-theory originating descriptors and topological descriptors have been developed over the years to describe fullerene stability, with moderate success and with implementation in a range of softwares[1]. Fullerene stability doesn't correlate with the number of resonant or Kekule structures either, which is the case in benzenoid hydrocarbons: among the 1812 isomers of C60, the most energetically stable one is 20th , while the most unstable one is 1st in the ranking by number of resonance structures [1]. Certain hydrogenated forms of C60 fullerenes, including C60H36 and C60H60, have been experimentally observed as stable. In the context of kekule structures of buckminster fullerene, hydrogenation of bonds can be thought of as reduction of numbers of resonant structures at certain locations [2].In out preliminary findings, DFT energies of variously hydrogenated buckminster fullerenes, surprisingly correlate stability of partially hydrogenated structures with the number of resonant structures. The most energetically stable hydrogenation patterns, seem to be when hydrogen atoms are added in pairs. The correlation is present across various level of theory. Current preliminary TDDFT data [3], is the starting point for upcoming calculations that explore excited states of hydrogenated fullerenes at higher levels of theory.

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Targeted enrichment of the training dataset as a path to more accurate predictions

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Machine learning is routinely used to screen of big databases of chemical compounds in search of molecules matching the desired quality [1, 2]. Main limitation is lower and often unpredictable accuracy of the prediction in comparison to more rigorous computational methods. This accuracy is influenced by multiple factors, where the quality of the training data set plays a crucial role [3]. The size of even large training set is tiny compared to the vastness of the chemical space. Moreover, the interesting compounds are generally underpopulated in a random selection and therefore not well predicted. This can be mitigated by more a targeted approach in the training set selection. Iterative methods of augmenting training dataset have shown promise [2]. Here only one step will be investigated with respect to various selection criteria. Neural network have been constructed using the SchNetPack 2.0 [4] program package and trained on docking scores towards the main protease (Mpro) of the coronavirus SARS-CoV-2 provided by the AutoDock Vina 1.2.2 software [5, 6]. Multiple aspects of prediction accuracy and prediction error were considered. Prediction errors are evaluated as a mean square error and mean absolute error of the whole test dataset. Special focus is dedicated to change in recall and precision of the predictions.

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Computational Insights into Photochromism of Triarylhydrazones

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Hydrazones represent an important class of photochromic compounds exhibiting bistable photoswitching which stems from exceptionally high thermal stability of the metastable isomer, fast photoisomerization, resistance to hydrolysis, facile synthesis, and easy skeleton modularity [1,2]. Recently, our group reported the photochromic behavior of a new subclass of hydrazone-based photoswitches – triarylhydrazones (TAHZs) [3,4]. These preserve most of the attractive features of other hydrazone-based photoswitches, but typically exhibit higher molar absorptivities and operate under light above 365 nm. First designed TAHZs involved pyridine/quinoline derivatives. Combining quantum-chemical calculations and ultrafast transient absorption spectroscopy measurements, the photoswitching mechanism was elucidated. Whereas the skeleton based on the pyridyl hydrazine ring led to an excellent thermal stability of >200 years and efficient photochemistry, 2-(naphthoyl)quinoline analogs were shown to operate at the desired longer wavelengths, preserving the thermal stability of several years of the parent systems. Nevertheless, most of the designed TAHZs displayed $Z \rightarrow E$ quantum yields (QYs) below 1%, which was attributed to competitive non-radiative pathways, including the excited-state intramolecular proton transfer (ESIPT) from the –NH group to the heterocycle. The potential of TAHZs was further enhanced by designing naphthoyl-benzothiazole hydrazones that balanced the most beneficial features of previously reported TAHZs, although the increase QYs of $Z \rightarrow E$ photoisomerization was not observed despite the anticipated weakening of an intramolecular H-bond [5].

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Density-based basis-set correction within local approximations

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In electronic structure calculations, coupled-cluster singles and doubles with perturbative triples [CCSD(T)] is considered the "gold standard" for weakly correlated systems. Its accuracy, however, comes at a high computational cost, primarily due to slow convergence with respect to the size of the one-electron basis set. Recently, Toulouse et al. [1] proposed the density-based basis-set correction (DBBSC) to address missing short-range correlation effects arising from the incompleteness of the one-electron basis set. DBBSC employs a short-range density functional with a range-separation function, complementing the long-range interactions accurately described by wave function theory, and automatically adapts to the spatial inhomogeneity of basis-set incompleteness (BSI).

DBBSC has been implemented [2] in our efficient local natural orbital-based CCSD(T) [LNO-CCSD(T)] scheme. Here, the range-separation function is decomposed into contributions from localized molecular orbitals, evaluated within compact, restricted domains. Additionally, the complementary auxiliary basis set (CABS) correction, significantly enhancing Hartree–Fock energy accuracy, is employed, relying on local density fitting approximations. Errors arising from local approximations have been thoroughly examined, and efficient prescreening techniques have been introduced to compress the numerical quadrature. Representative examples involving up to 1000 atoms illustrate the efficiency of the method. Numerical results confirm substantial reductions in BSI errors, often below 1 kcal/mol compared to reliable LNO- CCSD(T) complete basis set references when using double-ζ basis sets. The DBBSC and CABS corrections only moderately increase computational time, making DBBSC-LNO- CCSD(T) highly efficient for large-scale computations.

Furthermore, DBBSC has been extended to double-hybrid (DH) functionals [3], achieving accuracy comparable to recently proposed explicitly correlated (F12) DH methods [4] but with significantly lower computational demands. Real-life examples show only a 30% increase in computational time compared to conventional DH calculations without additional memory usage. Thus, DBBSC-DH presents an attractive alternative to DH-F12 functionals for extended molecular systems.

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Explicitly correlated geminal-based perturbation theory

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Wavefunctions built from two-electron units (geminals) are a straightforward generalization of the Hartree–Fock model. Incorporating intra-pair correlation at the reference level, they can be a practical tool for describing static correlation. Recent reports [1] show the potential of combining pair-function based methods with explicitly correlated corrections. In this work, we employ a strongly orthogonal geminals' model, termed SLG, which has an efficient polynomial scaling, serving as a low-cost alternative to complete active space based methods. On top of the multideterminantal SLG reference, dynamic correlation is accounted for by perturbation theory (PT) at second order via a Dyall-like Hamiltonian acting as the zero-order operator [2]. As a consequence of the structure of SLG and the associated zero-order Hamiltonian, the PT equations decouple into smaller problems, facilitating an efficient solution scheme.

An explicitly correlated (F12) correction is added to SLGPT to improve the description of dynamic correction and enhance convergence with respect to the basis set. The resulting SLGPT2-F12 scheme [3] will inherit the fragmented structure of the SLGPT2 method, thereby increasing the computational cost only insignificantly. As illustrative examples, the SLGPT2-F12 approach is applied to singlet-triplet splittings in small molecules.

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A Computational Study of Hydrogen Adsorption on Nickel-Modified Borophene

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This study explores nickel-decorated β_{12} borophene surface using DFT to evaluate its potential for hydrogen storage. Among four possible H_2-Ni interaction modes (side-on [1], end-on [2], H_2 dissociation [2] and H_2 spillover[3], [4]), side-on adsorption is most favorable.
All calculations were performed using the CRYSTAL17 software package [5] with the PBE [6] and PBE0 functionals, employing the pob-TZVP basis set. Grimme's GD3 dispersion correction was applied to enhance the treatment of weak interactions in the PBE0 functional.
Initially, a single hydrogen molecule was adsorbed onto the Ni-decorated β_{12} borophene in a side-on configuration. The reaction energies computed with both functionals are comparable, with minor differences in adsorption strength and negligible variations in geometric parameters.
Successive addition of H_2 molecules (up to seven) reveals that the average adsorption energy per molecule falls within the optimal range (15–60 kJ mol^{-1}) for practical hydrogen storage, starting from the adsorption of the second molecule. As hydrogen loading increases, Ni–borophene and Ni–H_2 distances also increase, indicating a weakening interaction. Notably, the H–H bond of the side-on adsorbed molecule slightly contracts, while the average H–H bond length remains nearly unchanged.
Mulliken charge analysis indicates that charge transfer to each hydrogen molecule decreases with higher hydrogen coverage, suggesting reduced electron donation as the surface becomes saturated. Future work will involve investigating β_{12} and χ_3 borophene surfaces decorated with various metals (e.g., Li, Na, K, Fe, Co, Cu, Zn) to identify trends in adsorption behavior and structural modification. Focus will be given to Ni-decorated surfaces and additional DFT functionals, as well as the study of Ni clustering on pristine β_{12} borophene.

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Exploring the Regioselectivity of Diels-Alder reactions of new 2,6-disubstituted benzoquinones by means of quantum chemistry

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Diels-Alder reactions of 2-methyl-6-substituted-*p*-benzoquinones were studied using quantum chemical calculations. The effect of nineteen substituents, including halomethyl, alkyl, vinyl, ethynyl, nitrile, trifluoromethyl, methoxy, cyclohexenyl, phenyl, and trifluoromethoxyphenyl groups, on the reaction barriers was explored by the B3LYP-D3, M06-2X, and DLPNO-CCSD(T) methods. Gibbs free activation energies were compared for the two regioisomeric products experimentally observed in the reaction mixture. A linear dependence of the calculated barrier difference ($\Delta G^{\ddagger}$**b** – $\Delta G^{\ddagger}$**a**) on the natural logarithm of experimentally observed product ratio, ln(**a**/**b**), expected based on the Eyring equation, was semiquantitatively fulfilled. Activation barriers were further analyzed in terms of the underlying deformation and interaction energies. The difference in deformation energies of transition states corresponding to the two regioisomers ranges from −8.0 to +8.0 kcal mol^{-1} and is directly proportional to experimental ln(**a**/**b**) values. Differences in interaction energies between regioisomeric transition states are, in comparison, significantly smaller.

COMPUTATIONAL MODELLING OF GLUTAMATE DEHYDROGENASE IN CROWDED ENVIRONMENT WITH FOCUS ON THE ACTIVE SITE

Daniel Myšák

Krupičková Pluhařová Eva, Mgr. Ing., Ph.D.

Living organisms regulate their life functions by biocatalyst called enzymes. Enzyme's activity is very sensitive to its surrounding which allows the cells to quickly react and change metabolism. Cell's interior contains large variety of macromolecules, thus it is crowded. However, most of the in vitro experiments are made in simple aqueous buffer. That is why we focus on the influence of the crowded environment.

Using all-atom classical molecular dynamics, we simulated Glutamate dehydrogenase (GDH), an important enzyme at a metabolic branching point in all living organisms [1]. Our model systems contained a bovine GDH trimer (Fig. 1) under various conditions (pH, molecular crowding agents such as glucose or dextran) [2]. We observed that the active site residues and substrates in the active site (Glutamate, Norvaline) are flexible. Interestingly, under certain conditions substrates spontaneously left the active site in two directions. Thus, by applying external force on the substrate we developed a protocol of pulling in a well-defined way. The results were discussed in the context of our previous simulations and available experimental data. These observations may help in explaining how enzymes behave in the crowded cellular environment and how such conditions affect substrate binding.

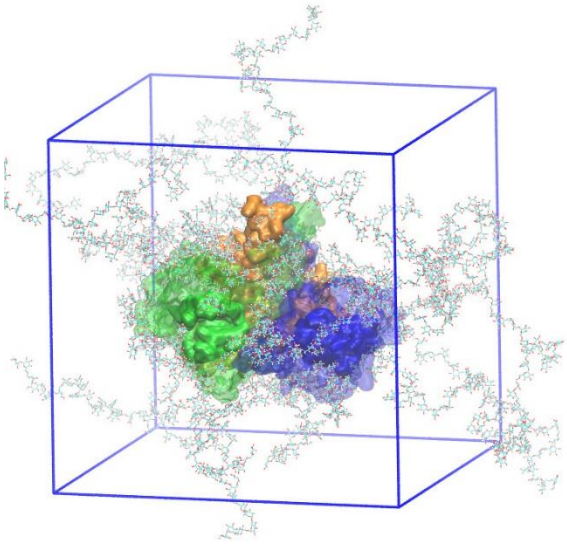

Figure 1: Simulation box with GDH trimer and displayed dextrans from the solvent.

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Identification of distinct spin transmission pathways in *acac* ligand coordinated to Ru(III)

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Assignment of solid-state NMR signals of open-shell coordination compounds remains a challenging task for computational chemists [1]. In this contribution we are analyzing hyperfine shifts of ^{13}C in acetylacetonate ligand (*acac*) coordinated to Ru(III). Single unpaired electron breaks the D_3 symmetry of $Ru(acac)_3$ complex which is reinforced by crystal packing in solid state. Thus, nonequivalent position of the ligand moieties with respect to paramagnetic Ru center allows us to distinguish two mechanisms of spin density propagation.

In order to separate and describe in detail these two pathways, we have designed and synthesized C_{2v} model systems Ru(*acac*)$Cl_2(NR)_2$ with only one *acac* ligand differing in the relative position of remaining paired ligands (*cis* and *trans*). A distinct location of Cl ligands with respect to Ru-*acac* ring determines the orientation of single occupied molecular orbital and subsequently induces fundamentally different patterns of spin density on *acac* atoms. The resulting contact hyperfine shifts calculated at DFT level are being interpreted based on atomic spin population and structure of frontier MOs. Special attention is paid to the role of molecular geometry and correlation effects.

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Electron force field as a gateway to X-ray photochemistry?

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X-ray photochemistry is an emerging field that investigates the use of high-energy photons to control molecular processes. While experimental capabilities have seen significant advances, theoretical methods have struggled to keep pace due to the complexity of phenomena such as Auger decay, multiple ionization, ultrafast electron scattering, and solvent-mediated reactivity. Unlike conventional UV-Vis photochemistry, where excitation typically occurs in isolated chromophores, X-ray-induced dynamics generally originate within the bulk medium, initiating cascades of reactive events. Time-dependent quantum chemistry approaches such as real-time time-dependent density-functional theory (RT-TDDFT) offer a rigorous framework but are limited by computational cost, restricting their application to small systems and short timescales. As a computationally efficient alternative, the electron force field (eFF) method, introduced by Su and Goddard, incorporates quantum effects into classical molecular dynamics by representing electrons as Gaussian wave packets coupled to classical nuclei [1]. To address the limitations of the original spherical-packet formulation, the eFF2 method explicitly assigns s and p orbital character to each electron [2].

In this study, we benchmark eFF2 on prototypical problems in water radiation chemistry, calculating electronic stopping powers for protons and heavier ions (He^{2+}, Li^{3+}), impact-parameter-resolved fragmentation cross-sections in water, and femtosecond-scale dynamics following single and double ionization of water monomers and dimers. Results are compared to experimental data and higher-level simulations where available. The eFF2 model qualitatively captures stopping power curves, including the low-velocity regime where linear-response theory fails, as well as proton transfer in singly ionized dimers and Coulomb explosion in doubly ionized dimers. However, it currently falls short in describing chemical reactivity, such as fragmentation cross-sections, and dynamics in doubly ionized monomers. These findings demonstrate that, while inevitably an exploratory approach, the eFF2 formalism offers a reliable starting point for investigating the ultrafast cascade of processes initiated by ionizing radiation, requiring further validation by more advanced theoretical methods.

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Structure and dynamics of concentrated dextran solutions by molecular dynamics simulations

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Dextran is a water-soluble homopolysaccharide consisting of D-glucose monomeric units. It has a broad range of applications in food industry, cosmetics, medicine or research laboratories. [1] There, it is used in chromatographic matrices or as a crowding agent mimicking the densely packed cellular environment. [2] Thus, rheological properties of dextran solutions as well as the polymer conformation, radius of gyration or hydrodynamic volume are of great practical importance. Various experimental techniques have been employed to address these questions, but less attention has been paid to the structure of dextran aqueous solutions at the molecular level.

Our recent molecular dynamics study with all-atom force fields [3] is the first application of this approach to concentrated dextran solutions. The simulated average radius of gyration of dextran chains agrees well with experimental findings, while trajectory analysis reveals diverse conformations of the polymers, ranging from compact to extended. Such conformations, determined by the relative orientation of neighboring glucose units, cannot be approximated by a simple spherical model. Here we investigate how commonly used buffer at various pH values influences the structure and conformations of the dextran polymer chain. Trajectory analysis shows that buffer molecules interact with different parts of dextran depending on pH. Obtained results improve our understanding of concentrated solutions of this widely used sugar polymer and macromolecular crowding agent.

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Temperature-Dependent Conformational Equilibrium of RNA 2'-OH Groups in Molecular Dynamics

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The orientation of the 2'-OH group plays an important role in the conformational equilibria of RNA, particularly in non-canonical motifs. Stabilizing signature interactions are often associated with a hydroxyl group being oriented toward the nucleobase. In stem regions, however, the equilibrium is more nuanced. NMR studies have arrived at conflicting conclusions [1], some supporting a base-oriented conformation [2], while others favor a torsion directed toward the backbone [3]. A recent joint X-ray and neutron diffraction study resolved the ambiguity of the 2'-OH orientation in the Sarcin-Ricin Loop by direct observation of hydrogen positions at low temperature.[4]

We use low-temperature molecular dynamic simulations to reproduce these conformational equilibria and study their dependence on temperature. Our goal is to reconcile contradictory experimental findings and evaluate the ability of current OL3 AMBER force field to accurately describe the conformational preferences of the 2'-OH group in RNA.

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Improving the performance of Double Hybrid functionals through regularization

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The second-order perturbation energy expressions (i.e., MP2 and GL2) have been a workhorse for quantum chemistry methods for many years. It has been widely utilized in the post-Hartree-Fock (post-HF) calculations and Kohn-Sham density functional theory (KS-DFT) to define various classes of functionals, e.g., Double Hybrids (DH). Although the list of successful applications of the MP2 method is quite long, it suffers from many limitations, like divergence in the cases where HOMO-LUMO energy gap closes, metallic systems, and large $\pi - \pi$ stacking systems.

In this work, we analyze several possible forms of regularization of MP2/GL2 energy expression in the context of post-HF and KS-DFT calculations to show the advantages and disadvantages of these formulas. Our analysis concentrates on model systems where standard second-order energy expression fails, i.e., stretched H_2 molecule, Hook's atom model, and homogeneous electron gas. We also present results for representative thermochemistry data sets from GMTKN55 benchmarks, which represent overall essential chemical properties. We demonstrate some numerical results proving that none of the investigated regularization schemes fully resolves all known problems related to the second-order correlation energy expression. However, we also show that there exist interesting candidate variations of MP2 which lower the errors in both in post-HF and KS-DFT calculations.

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Redox Behavior and Biomolecular Targeting of Acacetin-Cu(II) Complex: A DFT, Spectroscopic and Molecular Modeling Approach

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Acacetin (AC), a natural flavonoid, exhibits redox-sensitive bioactivity that is influenced by metal ion interactions. This study investigates the effect of binding of AC with Cu(II) ions using UV–Vis, EPR spectroscopy, and Density Functional Theory (DFT) calculations. DFT calculations confirmed stable complex formation and provide insights into its electronic structure. [1] Although AC acts as a potent $ABTS^{\bullet+}$ radical scavenger, this activity is influenced by Cu(II) coordination. In Fenton-like systems, excess AC decreased hydroxyl radical generation, as shown by EPR spin trapping. DNA interaction studies were performed with the intention to study binding to calf thymus DNA, which can be enhanced by Cu(II) coordination. [2] Electronic absorption titration, as well as in silico methods based on molecular docking protocols and molecular dynamics simulations confirmed the effective binding of AC to CT-DNA, strength of which is further enhanced by the presence of Cu(II) ions. Molecular docking and molecular dynamics (MD) simulations showed that the Cu(II)-AC complex induces partial DNA unwinding, suggesting significant structural impact. Fluorescence studies with human serum albumin (HSA) indicate that both AC and its complex may be efficiently transported in biological systems. [3] Molecular docking has been employed in an attempt to identify correct HSA binding site. The higher precision of MM-GBSA, as compared to molecular docking, while showcasing shortcomings of *in silico* approaches were assumed. Overall, this integrative approach combining spectroscopic techniques, DFT, molecular docking, and MD simulations provides mechanistic insight into how metal coordination alters the bioactivity of flavonoids like acacetin.

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Excited State Molecular Dynamics Simulation of Silaethylene including Spin-Orbit Coupling

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Abstract:

The non-adiabatic dynamics of molecules with photoexcited π-bonds is highly intriguing, involving a complex interplay of torsion, pyramidalization, and hydrogen transfer as they progress to the conical intersecting seam, which facilitates a transition to the electronic ground state. Including the spin-orbit interactions and triplet states into the picture can uncover additional new effects and behavior. Silaethylene ($SiCH_4$) is an example of molecule with polar π-bonds [1]. In this study, we carried out on-the-fly Tully's Fewest Switches Surface Hopping (TFSSH) to investigate the photodynamics of $SiCH_4$ with non-adiabatic (NAC) and spin-orbit coupling (SOC) [2,3]. We employed MR-CISD to compute the two lowest lying singlets (S_0 and S_1) and one triplet (T_1) state. The TFSSH trajectories were initiated on the lowest optically bright singlet excited state (S_1), modeling an optical excitation, and propagated for 500fs. Analysis of the simulation reveals that due to the SOC, an H transfer from Si to C and vice-versa can occur, leading to local minima with CH_3SiH and SiH_3CH diradical structures. Particularly the CH_3SiH isomer is energetically very close to the reactant and it thus indicates that a photoisomerization after excitation to S_1 can occur via a mechanism not available when restricting the simulation to singlet states only.

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Isobutanol to 2-butoxide on (100) surface of ferrierite: Insights from ML-accelerated AIMD

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The ever more severe environmental concerns create an urgent need to find viable sustainable energy resources to produce bio-based molecules used in industry. Relevant candidates in this context are linear butenes, which can be obtained from the dehydration of bio-alcohols and then used as reactive precursors for the synthesis of bio-polymers. In our previous theoretical studies [1, 2], multiple reaction pathways for the catalytic transformation of butanols into linear butenes over zeolite chabazite were explored, revealing alcohol isomerization and synchronous isomerization–dehydration reactions as key steps in the formation of linear butene products under experimental conditions [3]. Moreover, the relatively modest size of the simulation cell (85 atoms) allowed for the explicit inclusion of thermal effects through constrained ab initio molecular dynamics (AIMD) simulations, which revealed that the isomerization to butan-2-ol and the dehydration–isomerization reaction to but-1-ene proceed via a common transition state. However, a recent experimental study [3] on zeolite ferrierite has demonstrated that isobutanol exhibits limited diffusion into the interior of the bulk catalyst, while dehydration reactions predominantly occur at active sites located on the external surface. Since simulating the external surfaces of zeolites requires the use of very large structural models, their AIMD simulations were until recently prohibitively time-consuming and therefore rarely performed. This problem can be solved by accelerating the simulations using machine-learned force fields (MLFF) [4]. In this work, we use this approach to obtain fully anharmonic free energies of activation for selected reaction pathways of isobutanol to linear butenes on the (100) surface of ferrierite. A detailed comparison of the mechanisms and kinetics of the reactions at external surface with those in a bulk catalyst is presented.

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Structure-Based Identification of Musky Odorant Ligands Targeting Human Olfactory Receptor 5A2

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Human olfactory receptor OR5A2, a G protein-coupled receptor implicated in musky odorant perception, was structurally characterized using AlphaFold v2.3.1 [1] and employed in a comprehensive molecular docking study using GPU implementation of AutoDock [2]. Three sequential docking strategies were implemented: flexible macrocycle docking, hydrated docking with dummy water atoms, and a fully flexible docking model. Musky and non-musky compounds were docked and clustered into five receptor binding sites (A–E), with analysis focusing on binding site A, the presumed orthosteric pocket. The screening power of each model evaluated via ROC curves and AUC metrics across six musky compound families.
In addition to structure-based docking, machine learning classification models were trained using molecular descriptors of musky and non-musky in TensorFlow [3]. These models were evaluated using the same compound sets and ROC-AUC metrics, enabling direct comparison with docking-based approaches. This dual-framework analysis allowed us to benchmark the predictive potential of physics-based and data-driven models for musky odorant identification.

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The Reversal Spin-Flip (RSF) Approach Within pCCD for Open-Shell Quantum State

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In its standard single-reference formulation, the coupled-cluster model is one of the most accurate tools for describing dynamical electron correlation, as the hierarchy of approximations rapidly converges to the full configuration interaction solution. In the presence of quasi-degeneracies, the higher-order excitation terms are indispensable since low-level approximations do not provide a qualitatively correct structure of the wave function. The hierarchy of approximations based on the excitation level is broken down for systems featuring many correlated electrons, as found in complexes containing elements from the d and f block of the periodic table. Possible remedies dedicated to capturing strong electron correlation effects are, for instance, tailored coupled-cluster methods or simplified coupled-cluster approaches, where the cluster operator is restricted to electron-pair states. We will focus on a specific flavor of CC approaches where the amplitudes can be derived from geminal-based approaches like the pair coupled cluster doubles (pCCD) ansatz. Specifically, we will show how open-shell compounds can be modeled within pCCD-based approaches using spin-flip-style methods to describe the electronic structures of both closed- and open-shell molecules.

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Analyzing the nature of electron correlation in small metal clusters

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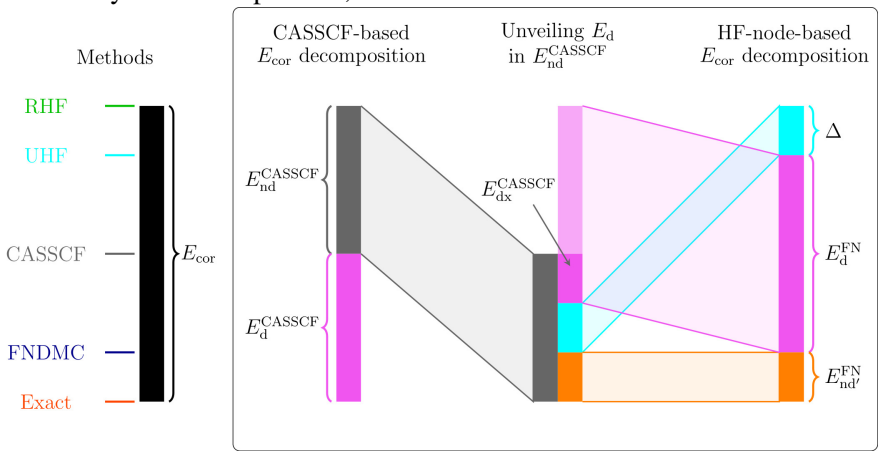
Atomically precise nanoclusters (NCs) are a class of nanoparticles with fascinating chemical and physical properties, which stem from their underlying electronic and geometric structure. Such precisely described structures give us the power to tune e.g. catalytic properties by hetero-atom doping. Ab initio modeling of transition metal-doped clusters usually rely on Density Functional Theory (DFT) calculations assuming a single-reference nature of the studied systems. We have recently developed a method [1, 2] for partitioning an exact electron correlation energy into the dynamic and non-dynamic components, which is based on the Fixed-node diffusion Monte Carlo (FNDMC) method utilizing the nodes derived from restricted Hartree-Fock Slater determinant. The proposed method allows for an unambiguous separation of electron correlation energies and will be applied to the analysis of the nature of electron correlation in small metal clusters.

Figure 1: Schematic representation of electron correlation energy decomposition into dynamic and non-dynamic components, based on HF nodes and FNDMC method



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Superalkali Clusters for CO_2 Activation: Role of Electronic Structure, Surface Charges and Ionization Potential

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We present a Density Functional Theory study of central- and surface-doped aluminum clusters with carbon dioxide. In this study we focus on how doping alters electronic structure, local surface charges, ionization potentials and finally how this affects catalytic activation of the CO_2 molecule. The crucial is the adsorption and activation of CO_2 on cluster surface, which is accompanied by charge migration resulting in the formation of bent CO_2^-. Among the strategies for CO_2 activation, one is to search for clusters with low ionization potential, so-called "superalkali" clusters able to promote charge transfer to CO_2. We have chosen Al_{13} as an ideal superatomic model cluster because of its uniform charge distribution and chemical inertness, which allow for the isolation and study of individual effects. Our results demonstrate that CO_2 adsorption is primarily driven by the existence of an active site with a partial positive charge on the cluster surface, which enhances the interaction with the CO_2 molecule and facilitates its activation in synergy with low ionization potential of the cluster. In a similar study we have shown that water adsorption on $Al_{12}X^-$ clusters is driven by cluster electron affinity and the reactivity of a cluster towards water dissociation can be tuned, controllably creating complementary active sites by targeted hetero-atom doping [1].

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Overcoming Bottleneck Operations in the Molecular Property Calculations in PyBEST with GPUs

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While the main driving force behind the development of the new graphics processing unit (GPU) hardware and software is deep learning algorithms, it also has an enormous impact on quantum chemistry, where GPUs allow the accelerated execution times of complex algebraic routines and open the way for studying larger molecular systems. To that end, we assess the performance of GPU assisted molecular property calculations in the PyBEST quantum chemistry software package [1, 2]. The unique features of PyBEST include a set of electron correlation methods based on the pair Coupled Cluster Doubles (pCCD) ansatz and its tensor contraction engine, allowing for off-loading the linear algebra operations to different external packages. Specifically, we focus on accelerating the PyBEST bottleneck operations on different GPU architectures (e.g., NVIDIA V100S and GH200) using PyTorch and CuPy. [3]

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Electronic structure of small organic molecules: DFT insights compared to experimental results

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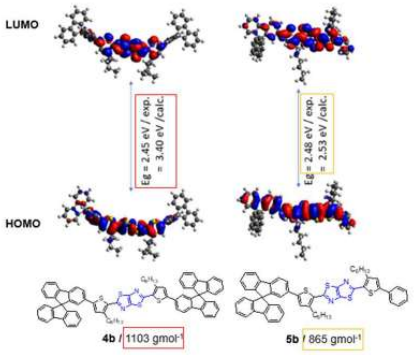
The development of small organic molecules that can serve as materials in OLEDs (organic light-emitting/electroluminescent diodes) and OPVs (organic photovoltaic devices) is urgent, as the dominant role remains in the use of conjugated oligomers and polymers [1]. Fabricating such structures is demanding from financial, time, and environmental perspectives [2]. Conversely, the design and synthesis of organic compounds with low molecular weights represent a time- and cost-effective process, with enhanced environmental protection due to, for example, the use of lower solvent volumes and reduced waste amounts. Using the standard Density Functional Theory (DFT), insights into the electronic structure and electro-optical properties of designed compounds are accessible before their synthesis. Since 2017 [3], we have been conducting this type of research. Our efforts in organic synthesis have recently culminated in success, as two of our small thiazolo[5,4-d]thiazole-based molecules have been applied as D–π–A linkers of the yellowish-green emissive layers in a laboratory-type of OLED [4]. In all our approaches toward that end, the DFT calculated electronic structure, band gaps and exciton binding are compared to experimental data according to cyclic voltammetry (CV), energy-resolved electronic impedance spectroscopy (ER-EIS) and UV-Vis spectroscopy [5-7]. The best match between DFT calculations and CV/ER-EIS results is achieved using the TPSSH/6-31G(d) or B3LYP/6-31G(d,p) exchange-correlation functionals and basis sets, respectively. We observed small differences between DFT-calculated frontier molecular orbital energy levels and experimental HOMO/LUMO values in our scope of synthesized compounds, particularly for those with lower molecular weights.



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Equation-of-motion coupled cluster theory for describing arbitrary conical intersections

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Balanced description of strong and weak correlations is still challenging in quantum chemistry. Among the models proposed for describing strong correlation, we have found that a modified version of the coupled cluster (CC) theory named CCSD0, which was rediscovered by Scuseria Group [1], is especially promising: For closed-shell systems, CCSD0 corresponds to one type of the projected Hartree-Fock (PHF) theories summarized by Hirao and Nakatsuji [2], which describe strong correlation in a single-reference manner by overcoming both the stability and symmetry dilemma. Moreover, the algorithms for CCSD0 are common to those for CC singles and doubles (CCSD). Once the F12 method is adopted as CCSD-F12 [3], the "CCSD0-F12" theory can describe both strong and weak correlations. Furthermore, once the equation-of-motion (EOM) scheme is adopted as EOM-CC [4], the "EOM-CCSD0-F12" theory can describe even S_1/S_0 conical intersections.

Despite such outstanding performance of EOM-CCSD0-F12 for describing electron correlations, when it comes to describing conical intersections between excited states, EOM-CCSD0-F12 is not free from the topological defect due to non-Hermiticity of the effective Hamiltonian of truncated CC theories. Apart from the computational expenses, the topological defect of conical intersections is the dominant reason why excited-state dynamics simulations conducted so far are almost never based on the CC theory [5]. Meanwhile, although unitary theories such as the algebraic diagrammatic construction (ADC) as well as the unitary CC theory describe topologically correct conical intersections, balanced description of electron correlations is not guaranteed at these levels of theory.

In this context, we propose an algorithm to diagonalize the CC Jacobian under the orthogonality condition derived by Kjønstad [6] that two roots must be orthogonal to each other in the subspace spanned by the roots. Once this algorithm has been adopted to EOM-CCSD0-F12 and the analytical energy gradient as well as the nonadiabatic coupling have been implemented, EOM-CCSD0-F12 will enable investigation of photochemistry with high accuracy which has not been achieved so far.

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Recent developments in second-quantization-based symmetry-adapted perturbation theory

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The poster contribution summarizes recent advancements in symmetry-adapted perturbation theory (SAPT) [1–3] developed by our group and our collaborators. All of the developments are connected through having one thing in common: they are all based on the second quantization formalism. [4, 5] The mentioned advancements include i.a., deriving and implementing first- and second-order exchange energy corrections (namely $E^{(10)}_{\text{exch}}$, $E^{(20)}_{\text{exch-ind}}$ and $E^{(20)}_{\text{exch-disp}}$) without the so-called *single-exchange* approximation in the second-quantized formalism [6]. This methodology was also extended to the third-order exchange-induction-dispersion energy $E^{(30)}_{\text{exch-ind-disp}}$ to obtain its unapproximated version. [7] Another noteworthy development is the extension of the SAPT capabilities to analytical derivatives for the calculations of interaction-induced properties (e.g., dipole moments) in the approach called propSAPT. [8] The current, most exciting effort is the development of a new SAPT-inspired method of calculating the dispersionless interaction energy through the use of the variational principle. This method called symmetry-adapted relaxation theory [9] (SART), is capable of obtaining the induction energy in the infinite order of the intermolecular interaction operator, accounting at the same time for the proper orbital relaxation effects. Eventually, the development of the code for symbolic derivations of second-quantized SAPT expressions from our group has proven to be highly beneficial in the work towards the mentioned advancements. [10]

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On the influence of halogen substitution on aromaticity in benzene-based systems

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Aromaticity is a fundamental concept in organic chemistry, yet a universally accepted and precise definition remains elusive. [1]. This problem stems from various perspectives, from which the aromaticity can be perceived. It is widely accepted that aromatic molecules must be cyclic, planar, fully conjugated and must contain 4n+2 π-electrons [2]. Additionally, it is universally and historically accepted that benzene is considered as the etalon of aromaticity. This results in various aromaticity indices that quantify aromaticity as deviations of several properties from those of benzene. This contribution is focused on both hypothetical and known halobenzenes analysing changes in aromaticity and selected electronic properties resulting from hydrogen-to-halogen substitution. Therefore, our studied group of molecules contains benzene, as well as its fluoro-, chloro-, bromo- and iodo derivatives. In addition, the intermediates of synthesis of hexafluorobenzene from hexachlorobenzene [3] were considered as well (Fig.1). The specific behaviour and limitations of the fluorination process are also considered.

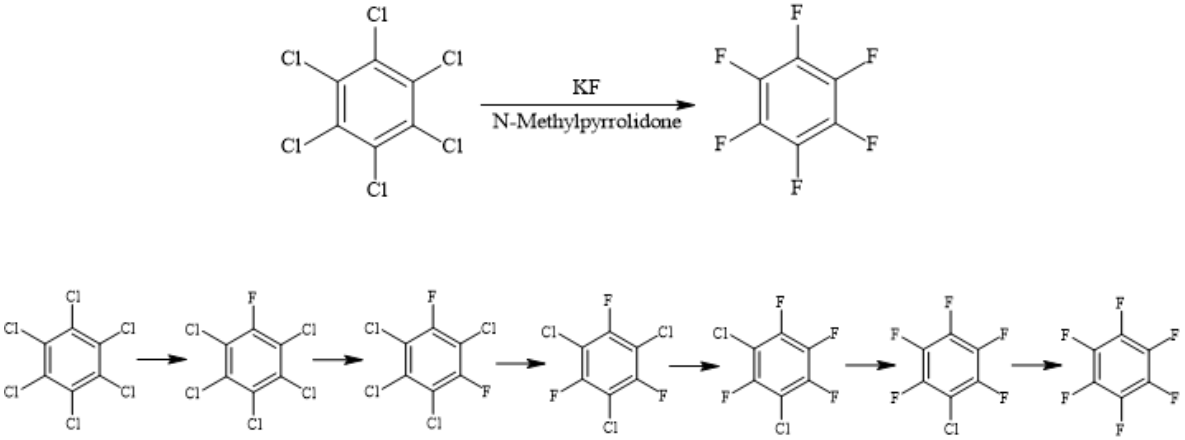

Fig.1 Experimental procedure of synthesis of hexafluorobenzene [3].

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Ultrafast correlation energy estimator

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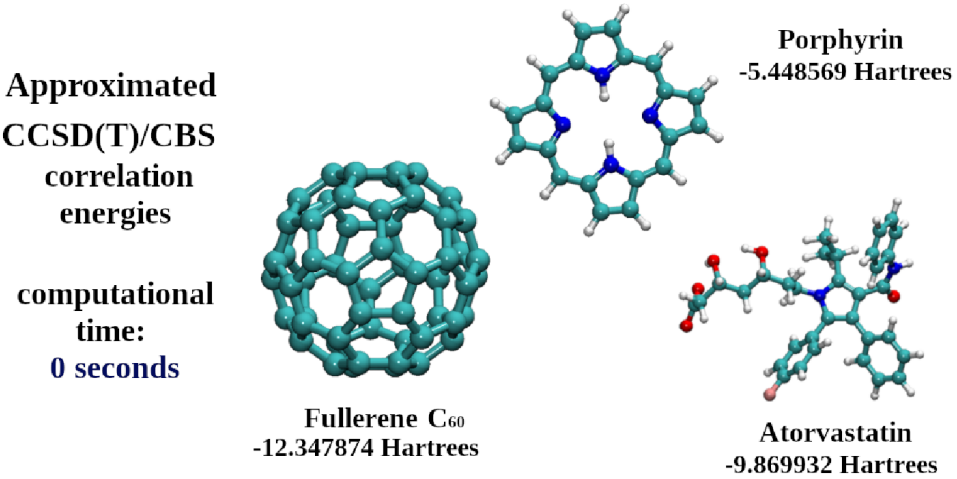
We introduce a novel computational method, Correlation Energy per Bond (CEPB), for efficiently estimating electron correlation energies with CCSD(T)-level accuracy at minimal numerical cost. By partitioning the molecular correlation energy into contributions from individual chemical bonds, the method is not size limited and can be applied to even large molecules, including proteins. Once these bond-specific energies are determined from independent calculations, they can be utilized across different molecular systems, making the approach both scalable and transferable. We demonstrated the effectiveness of the method on systems containing up to 650 atoms, showing highly accurate correlation energy predictions. Our analysis reveals intriguing regularities in correlation energies across different bond types, suggesting a relationship with the atomic size. At the current stage of development, CEPB can reliably assess the accuracy of other computational methods, such as DFT-based approaches or machine learning models, particularly for very large molecules where CCSD(T) calculations entail prohibitive computational cost. Therefore, CEPB serves as a practical alternative for generating highly accurate reference data. From a machine learning perspective, our findings highlight the number and types of chemical bonds as key molecular descriptors. Furthermore, we show that two-body contributions account for 99.5% of the CCSD(T)/CBS electron correlation, recovering MP2-level accuracy for reaction energies.



Implicit solvation models as an alternative for estimation of Clog *P* coefficient

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The log *P* coefficient is a well-known molecular parameter defined as the decimal logarithm of the ratio between the equilibrium concentrations in the aqueous phase (water) and the fatty phase (n-octanol). The log *P* is highly studied parameter in the early stage of drug discovery proccess reflecting the hydrophilic/lipophilic nature of examined molecule [1]. While appropriate hydrophilicity is associated with the solubility of a drug in water, sufficient lipophilicity is related to the transport of the drug across biological membranes. In view of this, an optimal value of log *P* can differ for individual drug based on its the site of action and the method of ingestion [2]. Importance of log *P* coefficient is emphasized by its inclusion in several sets of empirical rules (e.g., Lipinski [3], Ghose [4], Egan [5], …), which evaluate the druglikeness of potential drug candidates.

The time and financial demands of experimental measurement led to the development of computer-aided methods for Clog *P* (calculated log *P*) estimation. The most widespread *in silico* approaches use either additive manner (partial contribution of atoms/fragments) or methods based on topology. An alternative approach involves the use of quantum mechanics (QM) calculations. From another perspective, log *P* coefficient can be understood as a parameter describing thermodynamics equlibirum. This approach requires solvation Gibbs free energies in water and n-octanol, which can be computed using implicit solvent models (continuous medium) *via* calculations on the QM level of theory [6]. However, this raises questions about the accuracy of such an approach in predicting experimental log *P* values.

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