The van der Waals – London Discussions
Luxembourg 2025
October 15 – October 17

ABSTRACT BOOKLET

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Day 1 | Afternoon Presentations. Chair: Mirela Puleva

October 15th, 13:00 – 16:50 CET

Prof. Jean-Pierre Djukic

Predicting Reactivity from Density

Sara Figueireido de Alcantara Morais [a], Yann Cornaton[a], Eric Hénon[b] and Jean-Pierre Djukic[a],*
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13:10 - 13:50

Local non-covalent interactions may be informative a potential propensity of a molecule to undergo intramolecular reactions. In the Independent Gradient Model (IGM)[1] introduced by Hénon and coworkers, local non-covalent interactions are the weakest type of interatomic interactions. Yet, their assessment by this analytical method in crucial reactant complexes gives unique insights into the changes of electronic structure occurring during reactions occurring within the coordination sphere of a transition metal complex.[2,3] Extending the use of IGM to the analysis of full intrinsic reaction energy profiles gives access to detailed sequences of reaction events that otherwise could not be sensed.[4] These reaction events are all characterized by remarkable transient structures that correspond to key transformations involving electron density contributions from surrounding atomic centers. This new approach of reactivity dynamics is particularly useful for the analysis of concerted reactions relevant to catalysis.[4] It allows the monitoring of the electronic influence of non-central atomic centers in key events that was long inaccessible making the engineering of reaction more dependent on intuition.

1) J. Comput. Chem. 2023, 44(20), 1750. https://doi.org/10.1002/jcc.27123
2) Acc. Chem. Res. 2021, 54, 3828–3840
3) Synlett 2023, 34, 1169-1173
4) Manuscript(s) in preparation.

Prof. Berta Fernández Rodríguez

The Functional Group Correction approach versus machine learning

Departamento de Química Física, Facultade de Química, Universidade de Santiago de Compostela, Santiago de Compostela, Spain.

In recent work we developed the functional group correction (FGC) approach to correct the description of intermolecular interactions given by semiempirical quantum mechanical methods; in particular, we applied it to the PM6 and the GFN2-xtb approaches [1]. The new method is based on pairwise analytical corrections that work for specific functional groups and are derived from fits to interaction energy differences between the B3LYP-D3/def2-TZVP DFT values, taken as reference, and those provided by the particular semiempirical method [2]. Previously obtained corrections performed outstandingly well for alkanes and alkenes. In general, for the systems included in training and validation sets, the errors obtained with the PM6-FGC and xTB-FGC methods are within chemical accuracy. Considering the simplicity of the FGC approach and the speed of the involved calculations, its performance and outcome are promising, with results comparable to those provided by a recently developed state-of-the art delta machine learning (delta-ML) methodology, i.e. the PM6-ML approach [3], and significantly better than those obtained using the AIQM2 method [4].

1) E. M. Cabaleiro-Lago, B. Fernández, R. Rodríguez-Fernández, J. Rodríguez-Otero, S. A. Vázquez, J. Chem. Phys., 2023, 158, 124105.
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3) M. Nováček, J. Řezác, Journal of Chemical Theory and Computation, 2025, 21 (2), 678-690.
4) Y. Chen, P. O. Dral, 2024. Preprint on ChemRxiv:
https://chemrxiv.org/engage/chemrxiv/article-details/67042664cec5d6c1427a144f (2024-10-08).

13:50 - 14:30

Prof. Robert Pollice

Non-covalent interactions in molecular photocatalysis and photophysics

Stratingh Institute for Chemistry, University of Groningen, Groningen, The Netherlands

In this talk, I will introduce about our current work on developing a molecular string representation that not only captures covalent bonds and other strong interactions, but also noncovalent interactions. I will discuss the theoretical foundation and show application examples both from a cheminformatics perspective and with respect to machine learning models. As outlook, I will discuss future extensions towards a general framework allowing to create custom representations from any structure on demand.

14:30 - 15:10

Prof. Melanie Schnell

Structure and dynamics of weakly bound molecular clusters

Deutsches Elektronen-Synchrotron DESY, Hamburg & Kiel University, Kiel, Germany.

15:30 - 16:10

Rotational spectroscopy is a coherence technique known to determine the structures of molecules and molecular complexes in the gas phase in great detailranging from fundamental topics like proton transfer in microsolvated acids to astrochemistry. The structural information that can be deduced from the spectroscopic data provides an unprecedented molecular view on chemical processes, such as solvation and molecular recognition, governed by an interplay between hydrogen bonding and van-der-Waals interactions. For example, we studied complexes of polycylic aromatic hydrocarbons (PAHs), which are omnipresent in interstellar space, with an increasing number of water molecules to understand the initial steps of ice formation. We observe significant differences in the corresponding binding motifs for different PAHs, for example depending on the connectivity of the aromatic rings and the potential presence of hetero atoms. Furthermore, due to the high symmetry of the PAHs, rich intermolecular dynamics can be at play. In another example, we focused on water-driven dissociation of a single HCl molecule. In rotational spectroscopy, the nuclear spin of the chlorine atom is a sensitive probe of its electronic environment and thus its bonding situation. Consequently, our analysis allows us to precisely determine how many water molecules are needed for HCl to dissociate and provides insight into the intermolecular interactions of such complexes.

Prof. Wei Liu

Van der Waals effects in surface and interface chemistry

Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun, Jilin, China.

16:10 - 16:50

In the fields of catalysis and new materials research, surface and interfacial interactions play a crucial role in influencing various fundamental physicochemical processes. Among these, accurately describing many-body van der Waals (vdW) interactions remains a key challenge in achieving precise control over such processes. In this talk, I will present recent progress from our group in addressing this challenge: we developed a method to accurately describe many-body vdW forces, uncovering the fundamental nature of many-body effects, including screening, polarization, and their coupling with chemical bonding. Based on this approach, we elucidated the decisive role of screening effects in the formation of Langmuir precursor states, identified 56 new systems where physical and chemical adsorption coexist, and enabled the precise recognition of chiral molecules on defective surfaces, as well as the accurate prediction of reaction activity in prototypical electrocatalytic materials. This work opens new avenues for the rational design of advanced materials with tailored surface and interfacial properties, paving the way for further breakthroughs in energy conversion, catalysis, and materials engineering.

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2) C. Chen, Y. Ma, K. Yao, Q. M. Ji, W. Liu*, Enantioselective adsorption on chiral ceramics with medium entropy, Nat. Commun. 15 (2024) 10105.
3) J. Zhou, S. Yang, Y. Zhang, J.-C. Ren*, and W. Liu*, An effective descriptor for screening single-molecule conductance switches, J. Am. Chem. Soc. 146 (2024) 6962-6973.
4) M. Fang, J. Han, S. He, J.-C. Ren*, S. Li*, and W. Liu*, Effective screening descriptor for MXenes to enhance sulfur reduction in lithium-sulfur batteries, J. Am. Chem. Soc. 145 (2023) 12601-12608.

Day 1 | Poster Session.

October 15th, 16:50 – 18:00 CET

Dr. Margarita Shepelenko

Towards modeling laser-induced homogeneous ice nucleation from first principles

Poster 1

Margarita Shepelenko*, Leeor Kronik, Jan M. L. Martin, Leslie Leiserowitz

Department of Molecular Chemistry & Materials Science, Weizmann Institute of Science, Rehovoth 7610001, Israel

The phenomenon of ice nucleation from supercooled water, which has far-reaching ramifications for the living and nonliving world, generally occurs at a heterogeneous interface. Homogeneous ice nucleation, meaning far from pre-existing interfaces, is a challenge to induce and explore. Here we focus on laser-induced homogeneous ice nucleation reported by Nevo et al in 2020,(1) which we aim to understand from first principles. Our basic hypothesis is that the ice nuclei are formed without the help of the laser beam, but these ice nuclei are metastable. Interaction with the laser beam stabilizes the formation and growth of the nuclei. We started our computational study from ice XI, a proton-ordered orthorhombic polymorph of ice which has a triple point with hexagonal ice and gaseous water at (72 K, 0 Pa) and is stable below this temperature.(2) Ice XI is of interest for us owing the similarities between its crystal structure and that of hexagonal ice Ih. By virtue of orthorhombic-to-hexagonal cell transformation applied to of ice XI crystal structure, we obtained a proton-ordered ice structure in a hexagonal-ice-like cell and were able to compare the lattice energies and other parameters of interest of 'proton-ordered' and disordered hexagonal ice. In order to simulate an hexagonal ice (Ih) nucleus lying in liquid water, we made use of a model composed of 96 water-molecules(3-4) to generate a pseudo proton-disordered crystal of ice, surrounded by a water shell. This is work in progress and next we intend to study the effect of linear and circular polarized light on the ice nucleation process.

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2) Alan J. Leadbetter, Roger C. Ward, John W. Clark, Paul A. Tucker, Takasuke Matsuo, Hiroshi Suga, J. Chem. Phys. 82, 424–428 (1985).
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Prof. Eric Henon

A Practicable Measure and Spatial Visualization of Steric repulsion with Atomic Resolution

Poster 2

G. Hénon-Just [a], C. Lefebvre [b], A. Rajamani [c], H. Khartabil [c], J. Pilmé [d], S. Figueirêdo de Alcântara Morais [e], Y. Cornaton [e], J.-P. Djukic [e], E. Hénon [c]

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Steric repulsion, often regarded as a macroscopic manifestation of the Pauli exclusion principle, which prevents electrons with the same spin from occupying the same space, is experiencing renewed interest across the field of chemistry. [1,2] While its importance is widely recognized, visualizing where and how it occurs remains challenging. We introduce the Steric Exclusion Localization Function (SELF),[3] a novel tool that reveals steric interactions in three dimensions, requiring only a single quantum mechanical (QM) calculation. With SELF, chemists can see exactly where steric clashes happen in their molecules, quantify their magnitude, and identify which atoms contribute mostly to them. SELF transforms abstract QM concepts into intuitive 3D maps accessible through the user-friendly IGMPlot software. We demonstrate its power across diverse chemical systems: from understanding atropisomerism in pharmaceutical scaffolds to rationalizing selectivity in catalysis. Unlike traditional QM methods which condense the characteristics of steric effects into a single number, SELF provides visual insights that organic chemists can immediately interpret and apply. This approach bridges the gap between theory and practical chemical understanding, making sophisticated QM analysis accessible to the broader chemical community. We hope this tool will prove valuable for chemical design, research applications, and teaching steric effects. SELF tool is made available in the program IGMPlot http://igmplot.univ-reims.fr [4a] providing:

1. Three-dimensional visualization of steric interactions (coupled with IGM iso-surfaces[4b])
2. Quantification of local steric repulsion and integration.
3. Atomic-level decomposition of Pauli effects.
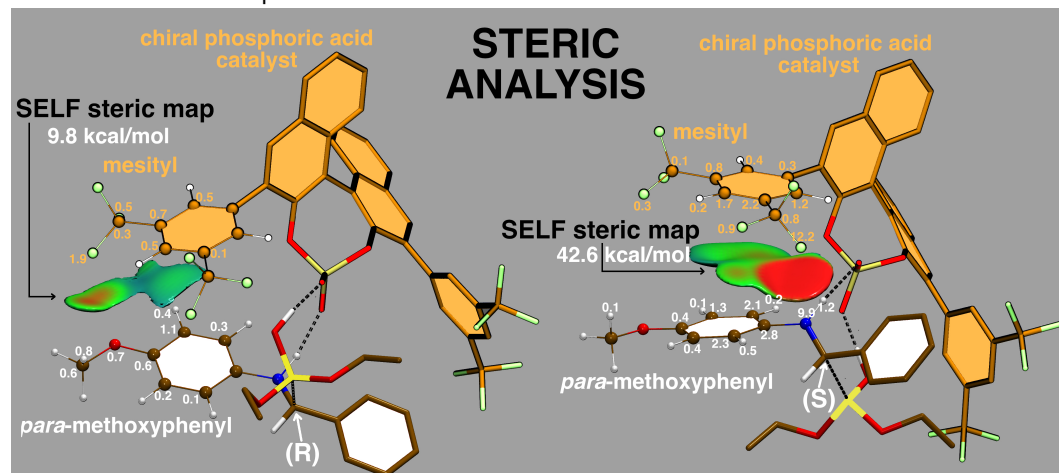
SELF is grounded in QM principles, providing a physically sound basis for steric analysis.

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2) M. M. Szczęśniak, G. Chałasinski, Front. Chem. 2022, 10, 858946.
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4) (a) C. Lefebvre, J. Klein, H. Khartabil, J.-C. Boisson, E. Hénon, J. Comp. Chem., 2023, 44, 1750-1766; (b) C. Lefebvre, G. Rubez, H. Khartabil, J.-C. Boisson, J. Contreras-García, E. Hénon, Phys. Chem. Chem. Phys., 2017, 19, 17928-17936.

Murillo H. Queiroz

Van der Waals effects in surface and interface chemistry

Murillo H. Queiroz[1], Suelen A. Santos[1], Tiago V. Alves[1], Roberto Rivelino[2]

Institute of Chemistry[1] and Institute of Physics[2], Universidade Federal da Bahia, Brazil

Poster 3

Aromaticity is usually linked to stability and electron delocalization in covalently bonded rings [1]. In this work, we explore how this concept can also appear in systems held together by H-bonds. We introduce the Harmonic Oscillator Model of Intermolecular Aromaticity (HOMIA) [2], a modified descriptor designed to measure aromatic behavior in cyclic H-bonded chains formed by HF, HCN, and HNC molecules. The HOMIA index is defined as: $\text{HOMIA} = 1 - (R_dim - 1/n \sum R_i)^2$ and captures deviations from ideal H-bond in the dimer due to cooperative effects. Using density functional theory (DFT) with dispersion corrections, we correlate HOMIA with key molecular properties, including bond lengths, cooperative binding energies, vibrational modes, and proton magnetic shielding. In larger rings ($n \geq 4$), cooperative effects become more significant, enhancing aromaticity through a combination of hydrogen bond shortening and covalent bond elongation. Our findings indicate that chains with fewer hydrogen bonds and an odd number of monomers tend to exhibit a more pronounced aromatic character, as revealed by structural and topological analyses. This work provides a fair model to analyze the aromaticity in non-covalent bonded systems.

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2) Queiroz, M. H, Santos, S. A, Alves, T. V, Rivelino, R. Submitted, 2025.

Bartosz Tyrcha

Interaction-Induced Properties as Analytical Derivatives of Symmetry-Adapted Perturbation Theory Corrections

Bartosz Tyrcha,* Tarun Gupta,* Konrad Patkowski,** and Piotr S. Zuchowski*

* Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in Torun, 87-100 Torun, Poland ** Department of Chemistry and Biochemistry, Auburn University, Auburn, Alabama 36849, United States

Poster 4

Interaction-induced properties, such as changes in dipole moments upon complex formation, are essential for a proper description of many phenomena related to intermolecular interactions, such as calculations of collision-induced absorption coefficients. This work presents an analytical framework for computing such properties directly based on symmetry-adapted perturbation theory (SAPT). The corrections for the one-electron interaction-induced properties are presented here in the first order of the molecular interaction operator. Calculations on selected polar and nonpolar dimers demonstrate that our approach reproduces the results of the finite-field treatment of the corresponding SAPT corrections. The approach proposes an insightful alternative for the computation of interaction-induced properties in weakly bound systems.

Andrea Buchwald

Exchange repulsion plays a crucial role in the structure of DNA base pair steps

Andrea Buchwald, Johannes Henrichsmeyer and Reinhold F. Fink
University of Tübingen

Poster 5

Intermolecular interactions between two stacked Watson-Crick base pairs AT or GC (base pair steps AA:TT and GG:CC) are considered as functions of certain structural parameters describing the local structure of DNA. These include twist (which leads to the helical structure of DNA), rise (the vertical separation of the base pairs), slide (a shift of one base pair along the long axis of the other), and propeller twist (the counter rotation of the nucleobases within the base pairs). Our calculations with symmetry-adapted perturbation theory (SAPT) expose exchange repulsion as the main structure-determining contribution to the total interaction energy. Dispersion and electrostatics have an additional influence, whereas induction plays a negligible role. The simple model of one «naked» base pair step, i. e. without backbone and/or solvent, works quite well in reproducing the sequence-dependent B-DNA structure. However, using methyl groups instead of hydrogen atoms at the positions of the backbone enhances the features of the PES.

Dr. Carlos R. Jacinto-Mejia

Transferable and Transparent Energy Decomposition-based Machine Learning Models for Computing Accurate Reaction Energetics

Carlos R. Jacinto-Mejia
University of Perugia

Poster 6

We present a transferable, interpretable, and modular machine-learning framework that enhances the accuracy of density functional theory (DFT) reaction energies using physically meaningful energy-decomposition descriptors. Reaction energies computed at the DFT level with standard basis sets are first decomposed into chemically intuitive contributions - such as kinetic and potential energy - which are then used to train a library of linear regression (LR) models. This includes a general-purpose model that reduces mean absolute percentage errors (MAPE) relative to gold standard CCSD(T)/CBS reference values by up to 63% compared to uncorrected DFT across extended benchmark sets. In parallel, a series of specialized LR models provide improved accuracy for specific reaction classes. A random forest (RF) classifier dynamically selects the optimal model for each case, pushing accuracy further and achieving MAPE reductions of up to 123%, all while maintaining full interpretability. In a rigorous out-of-distribution stress test on the WCCR10 dataset - containing transition-metal complexes absent from training - both the general LR model and the RF/LR pipeline retain robust performance. Compared to typical neural network models, which may suffer from generalization issues outside the training set, our framework shows stable performance outside its training domain.

Johannes F. Henrichsmeyer

The role of the nodal structure of π-orbitals in the interaction energy of π-stacked acene dimers

Poster 7

Johannes F. Henrichsmeyer, Michael Thelen, Andrea Buchwald, Keno Kraut, Benedikt Leyrer, Jihene Jerbi, and Reinhold F. Fink
University of Tuebingen

Our recently introduced model Molecular Orbital-Pair Contributions to the Exchange repulsion (MOPCE) [1,2] is applied to π-stacked acene dimers. Its key feature is the quantification of the contribution to the exchange-repulsion from each occupied molecular orbital-pair, consisting of one orbital of each monomer. To facilitate the analysis of the numerous contributions, they were grouped into three categories according to the type of orbitals involved ($\pi - \pi$, $\pi - \sigma$, $\sigma - \sigma$). With them, the role of the -orbitals can be easily investigated. Looking at a face-to-face arrangement in which a monomer is moved horizontally at a fixed vertical distance, it can be shown that the orbitals nodal planes perpendicular to the movement are reflected in the structure of the exchange repulsion and thus in the structure of the interaction energy calculated with the Symmetry Adapted Perturbation Theory (SAPT). By exploiting the dependence between the repulsion and the overlap of the orbitals, the repulsion can be transferred to the particle in the box model. It can thus be shown that the characteristic structure of the exchange-repulsion in acene dimers is indeed caused by the wave functions.

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Mambatta Haritha

Toward Accurate van der Waals Modelling: A Comparative Study of Empirical and Physical Approaches Using MoProSuite

Poster 8

Mambatta Haritha†, Benoît Guillot, and Christian Jelsch*
Université de Lorraine, CNRS, CRM2, F-54000 Nancy, France

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

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†Speaker * Corresponding author(s): christian.jelsch@univ-lorraine.fr
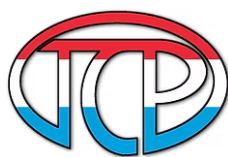
Martina Colucci

Coupled Cluster Analysis of Intermolecular and Intramolecular Interactions in Complex Systems: from Weak Interactions to Covalent Bonds

Poster 9

Martina Colucci
University of Perugia

Non-covalent interactions play a pivotal role in various areas of chemical research, including catalysis, materials science, and biochemistry. Nevertheless, their weak nature makes their experimental quantification challenging. In this context, theoretical chemistry offers highly accurate methods for their quantification and interpretation. Among these, the DLPNO CCSD(T) method, a local variant of the CCSD(T) method, together with the LED scheme, has been widely applied to complex systems containing hundreds of atoms. This approach allows to quantify and analyse interaction energies between an arbitrary number of fragments (molecules or functional groups) in a system from a single supramolecular calculation. It has found applications in catalysis, materials science and in the study of protein-ligand interactions.

In this work, we discuss our recent efforts to extend the LED scheme to covalent bonds, aiming to develop a more general decomposition framework applicable to both covalent and non-covalent interactions. This advancement addresses a key limitation of the current methodology and opens new avenues for analyzing chemical bonding in complex systems.

Dr. Yann Cornaton

Revealing Density Redistribution Events in Reaction Paths with the Independent Gradient Model

Sara Figueiarêdo de Alcântara Morai[1], Lucas Loir-Mongazon[1], Yann Cornaton[1], Eric Hénon[2] and Jean-Pierre Djukic[1]

[1] Laboratoire de Chimie et Systémique Organométallique, Institut de Chimie, UMR 7177 CNRS/Université de Strasbourg. [2] Institut de Chimie Moléculaire (UMR 7312), CNRS/Université de Reims Champagne-Ardennes.

Poster 10

The Independent Gradient Model (IGM) [1] is a theoretical chemistry tool which reveals interaction signatures through the analysis of the electron density gradient. It is used here to analyze in detail, along the Intrinsic Reaction Coordinates (IRC), the evolution of the electronic structure of a molecular system undergoing a concerted transformation. The case study reaction chosen here is the last step of a C–H bond functionalization reaction involving a doublet ground-state metallacyclic [Cp*Co(phpy)X]+ complex (Cp* = 1,2,3,4,5-pentamethylcyclopentadienyl, phpy = phenylenepyridine) in a product-releasing reductive elimination (RE) step. This step implies a selection of one-electron ligands –X (according to the Covalent Bond Classification).

The IGM-based atom-pair interaction Intrinsic Bond Strength Index (IBSI) [2] descriptor at the reactive center of the reactant complex is found to correlate with the activation energy barrier [3]. By the judicious choice of IGM descriptors, meaningful electronic changes occurring during a reaction can be revealed. Using the IGM-based interfragment interaction descriptor, it is shown that the Cp* ligand intervenes in the reductive elimination reaction as an electron density reservoir, providing density whenever the Co center undergoes transient coordinative unsaturation. Valleys and peaks of Degree Of Interaction (DOI) [4] at the cobalt center correspond to remarkable transient structures from which a host of electronic information can be extracted. The sourcing of the atomic contributions of peripheral atoms to the changes of DOI(Co) values gives an accurate insight into the role of the cobalt's ligands.In the case of the studied reductive elimination reaction, the IGM analyses of five highly sampled IRCs reveal that transition states (TS) do not correspond to peaks of DOI(Co), i.e., maxima of electron density sharing by the cobalt. The peaks of DOI closest to TS possess a sigma-complex-type structure. The monitoring of DOI(Co) and the atomic contributions also unveils the importance of secondary weak interactions [5].

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Dr. Almaz Khabibrakhmanov

Noncovalent Interactions in Density Functional Theory: All the Charge Density We Do Not See

Almaz Khabibrakhmanov, Matteo Gori, Carolin Müller and Alexandre Tkatchenko
Department of Physics and Materials Science, University of Luxembourg, 142a Avenue de la Faiencerie, L-1511, Luxembourg

Poster 11

Accurate determination of the electron density in molecules and materials enables direct access to interatomic forces via the Hellmann-Feynman theorem. However, density-functional approximations (DFAs) – the workhorse methods for electronic structure – often yield approximate densities that can be unreliable [1-3]. Here, we show that long-range van der Waals (vdW) dispersion interactions can significantly alter the electron density, exhibiting nontrivial scaling with system size and, in some cases, inducing polarization that exceeds that of the underlying semi-local DFA. To capture these effects, we introduce the Fully-Coupled and Optimally-Tuned Many-Body Dispersion (MBD@FCO) model, which computes the vdW-induced density by appropriately projecting to real space the collective fluctuations of coupled harmonic oscillators. We benchmark our method against accurate coupled-cluster singles and doubles (CCSD) densities for small molecules and extend its application to larger systems, including the S12L [4] and L7 [5] complexes and the Fip35-WW protein. Our findings underscore the potential limitations of post-hoc vdW corrections, highlight the significance of accurately resolving vdW-induced density changes in large (bio)molecules, and pave the way towards improved DFAs and density-based machine-learned force fields.

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Prof. Sergey P. Verevkin

How to quantify the dispersion forces in ILs?

Sergey P. Verevkin and Riko Siewert

University of Rostock, Institute of Technical Thermodynamics, Germany

Poster 12

Vapor pressures and vaporization enthalpies of tetraalkylphosphonium ionic liquids with [PF6]-, [NTf2]-, Cl-, and Br- anions have been measured using quartz-crystal microbalance and thermo-gravimetry. Chain-length dependences of the vaporization enthalpies have been established and used for validation of experimental data.

An empirical "step by step" protocol was developed for quantifying dispersion interactions in long-chained tetraalkylphosphonium-based ionic liquids by using vaporization energetics as a bulk property. Additionally, experimental vaporization enthalpies $\Delta_l^g H_m^\circ(298.15\,K)$ of n-alkanes (CH3-(CH2)$_n$-CH3) and tri-n-alkyl-phosphines (P(R)$_3$ with R = n-alkyl) were considered.

The idea of the first step is to remove alkyl chains completely, as they are the primary source of dispersion interactions. A linear chain-length dependence of vaporization enthalpy was developed: $\Delta_l^g H_m^\circ(298.15\,K) = Q \cdot N_C + Y$ for the [Pn n n m][PF6] and [Pn n n m][NTf2] series. It was logical to extrapolate these dependences to the imaginary case of $N_C = 0$. The intercept Y of the linear fit was referred to as the "residual" vaporization enthalpy, liberated from dispersion interactions through alkyl chains.

Physically, the quantity of the intercept Y differs between molecular and ionic compounds. It encompasses the contribution to vaporization enthalpy due to the anion itself, as well as the total Coulomb interactions between ion pairs in the liquid state.

Having established the intercept Y in each series by completely "cutting off" the alkyl chains from the real molecules, the second step toward quantifying dispersion forces due to van der Waals interactions of alkyl-chain segments was performed by subtracting the Y-values from the experimental vaporization enthalpy: $\Delta_l^g H_m^\circ((CH2)_n) = \Delta_l^g H_m^\circ(exp) - Y$ These $\Delta_l^g H_m^\circ((CH2)_n)$ values can be directly attributed to the dispersive interactions of alkyl chains in the liquid phase, assuming dispersion forces are negligible in the gas phase.

Prof. David Kreher

Single polyoxometalate-based nanoclusters characterized by infrared absorption nanospectroscopy

Poster 13

Juba Salhi[1], Michele Mattera[1], Imad Arfaoui[2], Jan Patrick Calupitan[1], Sandra Alves[1], Claire Troufflard[1], Céline Paris[2], Guillaume Izzet[1], Anna Proust[1], David Kreher[3], Guilhem Simon[2], Alexandre Dazzi[4] and Florence Volatron [1]

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Polyoxometalates are nanometric molecular oxides (general formula MxOyn- or XpMxOym- with M = WVI, MoVI, VV,. . . ; X = PV, SiIV, AlIII,. . .) with outstanding physical properties and great chemical versatility, widely studied in a large panel of applications in catalysis, biology, medicine, energy storage, information storage etc. In this context, here we present the full characterization, by combined and complementary techniques, of a sophisticated molecular assembly made of pyridine-terminated Keggin-type polyoxomolybdates (POM-pyr) linked to a zinc-phthalocyanine (ZnPc) deposited onto a layer of 1,3,5-tris[(E)-2-3,5-didodecyloxyphenyl)-ethynyl]-benzene (TSB-C12) self-organized on highly oriented pyrolytic graphite (HOPG). More precisely, first we will detail the different chemical engineering and supramolecular strategies we tested to try to reach such an advanced molecular system made of a layer of a POM-ZnPc complex deposited onto a layer of TSBC12 self-assembled on HOPG. Second and importantly, with this study we show that AFM-IR was decisive (compared to STM, i) insufficiently sensitive to detect nano-objects distanced of 50-100 nm from each other & ii) being problematics to characterize electrically charged, nanoiobjects) : indeed, AFM-IR yielded a particularly noteworthy result, as single POM-ZnPc complexes exhibited a tendency to insert into the pores of the TSB-C12 template, in a random manner, occupying isolated locations. To sum up, in this study, AFM-IR emerged as a crucial technique, with the potential to become a preferred method for the characterization of complex molecular layers. In our case, this technique proved that the hybrid POM preparation strategy, even though it does not guarantee their periodic organization, offers a promising approach to control surface handling of the nanoclusters. This work was accepted recently (Commun Chem 2024, 7, 299. https://doi.org/10.1038/s42004-024-01385-y).

Prof. Piotr Żuchowski

Single polyoxometalate-based nanoclusters characterized by infrared absorption nanospectroscopy

Poster 14

Piotr Żuchowski

Nicolaus Copernicus University

Symmetry-Adapted Perturbation Theory (SAPT) is renowned for its accuracy and interpretative power in modelling intermolecular interactions, but its scope has traditionally been limited to interaction energies. We present an extension of SAPT for interaction-induced properties, which we term propSAPT. This new framework has been tested on induced dipole moments in molecular and atomic dimers and further applied to compute differential interaction-induced electron densities. With propSAPT, we can also decompose density changes into specific, physically meaningful components—analogous to the way SAPT dissects interaction energies. This enables us to trace contributions from dispersion, polarization, and exchange effects to the overall property changes. Importantly, the interaction-induced modifications are expressed entirely in terms of monomer wavefunctions and response functions. The formalism is developed both within the Hartree-Fock framework and extended to Kohn-Sham density functional theory.

Dr. Riko Siewert

Quantification of dispersion forces and intramolecular hydrogen bonding strength in α,ω-alkanediols

Riko Siewert [1,2],*, Sergey P. Verevkin [1,2], Karsten Müller [1,2]
[1]University of Rostock, Institute of Technical Thermodynamics, Germany. [2]University of Rostock, Competence center °CALOR at the Department Life, Light & Matter.

Poster 15

Dispersion forces and hydrogen bonds are key contributions that influence the enthalpy of vaporization of organic compounds. α,ω-Alkanediols exhibit two distinct types of hydrogen bonding: intermolecular and intramolecular. While intermolecular hydrogen bonds typically result in increased boiling points, heat capacities, and enthalpies of vaporization, intramolecular hydrogen bonding tends to lower the enthalpy of vaporization by stabilizing specific molecular conformations in the gas phase.

However, determining the individual contributions to the enthalpy of vaporization, ΔH_{vap}, is challenging, as the vaporization enthalpy of diols is influenced by intramolecular hydrogen bonds, intermolecular hydrogen bonding, and dispersion forces:

$$\Delta H_{vap} = H_{inter-HB} + H_{dispersion} - H_{intra-HB}$$

The quantification of these contributions requires a multi-method approach, involving infrared (IR) spectroscopy, computational methods, group contribution techniques, calorimetry, and homomorph models. Each of these methods provides insight from a different perspective.

Quantum chemical calculations estimate gas-phase enthalpies of formation for both hydrogen-bonded and non-bonded conformers, using their difference to approximate the bond strength. Group contribution methods rely on experimentally measured gas-phase enthalpies of formation and compare compounds with and without intramolecular hydrogen bonds and similar dispersion forces.

IR spectroscopy can be performed either in the gas phase or in dilute solutions, with the latter requiring solvent effects to be considered. The homomorph approach bridges gas and liquid phases by correlating enthalpies of vaporization, accounting for both intra- and intermolecular hydrogen bonding as well as dispersion forces.

This study demonstrates that, despite differences in definitions and phase-specific considerations, it is feasible to assess the strength of intramolecular hydrogen bonding and dispersion forces in α,ω-alkanediols through a comprehensive, cross-methodological evaluation.

Dr. Dahvyd Wing

Approximating Pauli Exchange-Repulsion: A Transferrable Model Based on Electron Density

Dahvyd Wing and Alexandre Tkatchenko
Faculty of Science, Technology and Medicine, University of Luxembourg, 2 Av. de l'Universite, 4365, Luxembourg

Poster 16

Current approaches to modeling Pauli repulsion in molecular force fields for biological systems often rely on over 20 atom types to achieve chemical accuracy. The number of parameters in these approaches hampers the development of force fields with quantum-chemical accuracy that are transferrable across many chemical systems, as fitting procedures tend to conflate exchange-repulsion with other short-range effects such as charge transfer. We present a low-parameter, semi-classical model for exchange-repulsion derived from the electron density. This electrostatics-based model reproduces symmetry-adapted perturbation theory (SAPT) reference energies with chemical accuracy for a representative set of small organic molecules. Its minimal parameterization and high accuracy presents the possibility of fitting to high-level reference calculations while preserving transferability across chemical systems, offering a promising path toward high-accuracy, next-generation force fields.

Day 2 | Morning Presentations. Chair: Prof. Jean-Pierre Djukic

October 16th, 9:00 – 12:00 CET

Prof. Giovanni Bistoni

Predicting Reactivity from Density

Dipartimento di Chimica, Biologia e Biotecnologie, Università degli Studi di Perugia, Perugia, Italy

9:00 - 9:40

Local correlation techniques exploit the short-range nature of dynamic electron correlation to mitigate the inherent steep scaling of wavefunction-based methods. In this contribution, I discuss novel methods [1-5] based on local coupled cluster theory for studying dispersion effects on reactivity [6] and interactions [7] of large and complex chemical systems (Fig. 1). The family of local correlation methods offers a powerful toolbox for achieving both high accuracy and chemical insights simultaneously.
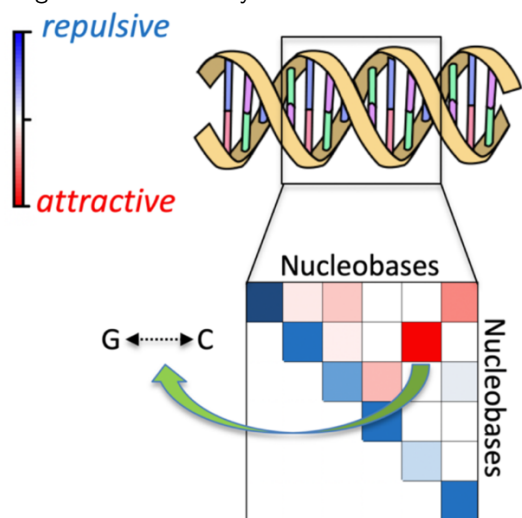
Fig. 1: Recent local coupled cluster study on a large DNA duplex model (1001 atoms, 13998 contracted basis functions) provided an in-depth characterization of the key inter- and intra-strand interactions responsible for the stability of human DNA[7].

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4) Gianluca Regni, Lorenzo Baldinelli, G. Bistoni, Submitted
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Prof. Maria Fyta

Assessing van der Waals interactions in hybrid systems made of biomolecules and materials

Taner Dogan, Lydia Spatz, Peijia Wei, Longlong Li and Prof. Maria Fyta
Computational Biotechnology, RWTH Aachen University, Aachen, Germany

9:40 - 10:00

VHybrid systems made of a biomolecular and a material part, typically, within an electrolyte solution are involved in complex interactions. An important component in these interactions are dispersion or van der Waals forces and are not always easy to handle and model. The strength of these interactions is strongly dependent on the molecular and material type and their relative arrangement. This rich dependence is not always sufficiently taken into account by interaction models. In order to understand these differences and assess the quality of respective models, we turn to density functional theory (DFT) and choose different schemes for van der Waals corrected exchange correlation (vdw-XC) functionals. Where necessary we complement the insights gained with those from atomistic simulations. As probes for the assessment of the vdw-XC functionals, we model two types of cases reflecting different interaction and bonding environments: (a) single amino acids placed within a graphene pore and (b) single amino acids and sugar molecules interacting with defective graphene. The interaction curves extracted from the respective DFT simulations are assessed providing important ideas towards the modeling of van der Waals interactions in hybrid bio/material systems with applications in protein detection and biosensing.

Dr. Martin Michael Müller

Protein-membrane interactions with a twist

Jordan Klein, Loréne Schad, Thérèse E. Malliavin and Martin Michael Müller
Université de Lorraine, CNRS, LPCT, France

10:00 - 10:20

To understand how a biofilament can interact with a lipid membrane, mesoscopic models are of particular interest. Within a framework of elasticity theory and geometry, two mechanisms have been proposed, which can induce membrane deformations due to a biofilament: the Twister and the Darboux torque mechanism [1]. Whereas the Darboux torque mechanism has been shown to explain membrane deformations by a polymer in several important biological systems, the Twister mechanism has been studied more carefully only recently, which has allowed for the development of a possible explanation for the membrane translocation of botulinium toxins [2]. In my talk I will present coarse-grained molecular dynamics simulations of a protein in interaction with a membrane. The protein is modeled as a cylinder stabilized by a tensegrity scheme, leading to an elasticity similar to that observed in real proteins. The Twister mechanism is induced by a hydrophobic helical strip displayed by the protein. The entire configuration space is explored by systematically varying the hydrophobic strip width, the twisting of the strip as well as the range of hydrophobic interactions between the protein and the membrane. The results are explained using a qualitative model based on the total hydrophobic moment of the protein.

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Prof. Ángel Martín Pendás

Non-covalent interactions in Real Space: Tracing Electron Correlation, Intermolecular Bonds, and Dispersion from the IQA Perspective

Facultad de Química, Universidad de Oviedo, Oviedo, Spain

10:40 - 11:20

A fundamental understanding of dispersion and other non-covalent interactions demands a framework that captures correlation energies with spatial resolution. Actually, many of the most successful computational frameworks devised to include dispersion corrections in a computationally efficient way, such as the DFT-D3(4), MBD, or XDM formalisms (see Ref. [1] for a survey), use some atomic partitioning. Here we show how to apply the Interacting Quantum Atoms (IQA) formalism [2,3], derived from real-space QTAIM [4] partitions, to investigate the nature of non-covalent interactions as well as the localization of electron correlation energy across a variety of molecular systems and intermolecular complexes. Leveraging high-level correlated wavefunctions, including CCSD(T) and near-exact FCI densities, we demonstrate that intra-atomic contributions overwhelmingly dominate the correlation energy, while interatomic terms provide chemically meaningful insight into both short-range and long-range correlation [5,6]. We show that the sign and magnitude of interatomic correlation energies offer a robust criterion to distinguish covalent from non-bonded or dispersive interactions, allowing a real-space reinterpretation of dispersion forces. A focused analysis of the dihydrogen triplet state across varying internuclear separations reveals that dispersion-like behavior emerges naturally in the interatomic correlation terms at large distances, while short-range contributions dominate near equilibrium. Our results propose the interatomic correlation energy descriptor as a reliable, position-space marker of dispersion, opening the door to intramolecular dispersion definitions within real-space frameworks. The combination of IQA energy decomposition with relaxed density matrices presents a powerful tool for dissecting non-covalent interactions in complex chemical environments and may inform the development of dispersion-aware real-space force fields.

Prof. Péter R. Nagy

Enabling gold standard level of accuracy in modeling complex noncovalent interactions between large (bio)molecules

11:20 - 12:00

Department of Physical Chemistry and Materials Science, Faculty of Chemical Technology and Biotechnology, Budapest University Of Technology And Economics, Budapest, Hungary

The accurate modeling of various ionic, aromatic, polarized, sigma-hole, surface, etc. interactions and especially their coupling to each other and to reactive processes remains challenging. We report advances in accelerating coupled-cluster (CC) methods and their convergence to the complete basis set limit (CBS), providing chemical accuracy even for large systems of complicated (single-reference) electronic structure. Our CC methods with state-of-the-art accuracy-over-cost performance include frozen and local natural orbital (FNO & LNO) approaches, optimized parallel closed- and open-shell implementations, linear-scaling MP2, LNO-CCSD(T), and general-order LNO-CC, as well as (so far conventional) CC gradients [reviewed in 1,2]. To improve basis set convergence, we developed an MPI+OpenMP parallel FNO-CCSD(F12*)(T+) code, a generally applicable floating orbital Gaussian basis (FOG) approach[2,3], and an LNO-accelerated DFT-based basis set correction[4]. LNO-CCSD(T)/CBS energies usually take about 1-2 order of magnitude more time than HF/hybrid DFT in the same basis set, have exceptionally low minimal memory and disk requirement (10s-100 GB), and are accompanied with robust uncertainty estimates. This makes them routinely applicable for molecules of 100s of atoms even with a single node.[1,2] We utilize the efficiency of LNO-CCSD(T) to model supramolecular and protein-drug/ion complexes, interactions in molecular liquids and crystals, as well as homogeneous, surface, and enzymatic catalysis, scaling up to 100s-1000 of CC-level atoms[1,2,4-8]. We report unique datasets consisting of 10-100 gold standard interaction energies for drug-side chain[6], and protein pocket-cation[7]/drug[8] interactions between real-life drug molecules of 40-80 atoms and pocket models of 100-300 CC-level atoms.

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2) MRCC program suite, www.mrcc.hu, JPCA 129, 2086 (2025)
3) JPCA 128, 10282 (2024)
4) JCTC 20, 7453 (2024)
5) Nature Communication 12, 3927 (2021), J Am. Chem. Soc. 145, 25372 (2023)
6) Puleva, Sanodas, Lőrincz, Charry, Rogers, Nagy, Tkatchenko (2025)
7) Zhao, Lőrincz, Berta, Henkes, Nagy, Tkatchenko, Vuckovic (2025)
8) Rezac, Lőrincz, Berta, Nagy (2025)

Day 2 | Afternoon Presentations. Chair: Sergio Suárez Dou

October 16th, 13:50 – 17:10 CET

Prof. Sason Shaik

A Gravitational-Like Behavior of Dispersion Interactions
Institute of Chemistry, The Hebrew University of Jerusalem, Jerusalem, Israel

We present computational results of many-body dispersion (MBD) interactions for more than 40 pairs of molecular and atomic species: hydrocarbons, silanes, corresponding fluorinated derivatives, pairs of CnHn cages, pairs which have multiple H—H contacts between the molecules, as well as pairs having interactions, and pairs of noble gases. The calculations reveal that the MBD stabilization energy (EDISP,MBD) obeys a global relationship, which is gravitational-like. It is proportional to the product of the masses of the two molecules (M1*M2) and inversely proportional to the corresponding distances between the molecular centers-of-mass (RCOM-COM). This relationship reflects the interactions of instantaneous dipoles, which are generated by the ensemble of bonds/atoms in the interacting molecules. Using Grimme's D4 corrected dispersion energy (EDISP,D4), we find that the data sets for EDISP,MBD and EDISP,D4 are strongly correlated (r2= 0.997). Based on valence-bond modeling, the intra- and inter-molecular dispersion interactions occur primarily due to the increased contributions of the oscillating-ionic VB structures which maintain favorable electrostatic interactions; the. [RC+:H+H :CR] and [RC:+H H:C+R] structures; R symbolizes a general residue. The local charges (on the C and H atoms) are propagated to the entire ensemble of bonds/atoms in the R residues, thus bringing about the gravitational dependence of dispersion.

1) D. Danovich, A. Tkachenko, S. Alvarez, S. Shaik, J. Am. Chem. Soc. 146, 311204 (2024)

13:50 - 14:30

Prof. Carlo Adamo

Extending nonempirical DFT models to noncovalent weak interactions
Chimie ParisTech, Institute of Chemistry for Life and Health Sciences, Paris, France

Weak non-covalent interactions remain a challenging area for most Density Functional Approximations, and the inclusion of empirical potentials has proven to be an effective way to address their limitations. Recently, we have proposed an alternative approach based on the coupling of a non-empirical double hybrid functional, PBE-QIDH, with a specifically developed basis set named DH-SVPD. This basis set was constructed using a dedicated procedure that does not involve any fitting to external reference data [1]. The results obtained across a wide range of benchmark datasets [2-4] demonstrate that our protocol, PBE-QIDH/DH-SVPD, provides interaction energies that are at least as accurate as those obtained with comparable functionals combined with large triple- or quadruple- basis sets and dispersion corrections. The rationale behind this performance can be attributed to improvements in the description of electronic molecular properties induced by our protocol.

14:30 - 14:50

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4) H. Li, E. Brémond, J. C. Sancho-García, Á. J. Pérez-Jiménez, G. Scalmani, M. J. Frisch and C. Adamo, Phys. Chem. Chem. Phys., 2024, 26, 8094–8105.

Prof. Majdi Hochlaf

On the mapping of multi-dimensional potential energy surfaces of weakly bound complexes of increasing size: state-to-the-art and challenges

14:50 - 15:10

Université Gustave Eiffel, COSYS/IMSE, Champs sur Marne, France

To treat the spectroscopy and dynamics of small and medium-sized weakly bound complexes, one needs an accurate multi-dimensional potential energy surface (mD-PESs). To date, first principles methodologies are available for the generation of such precise mD-PESs. They include Coupled Clusters methods extrapolated to complete basis set limit and where diverse non adiabatic and relativistic corrections are considered. Nevertheless, these methods can be used mostly for small molecular systems (i.e. di, tri or tetratomics) since their computational costs become prohibitive while increasing the size of the molecular systems. One needs alternative approaches where the computational cost is reduced without deteriorating the accuracy. For those purposes, several approaches were developed making use of explicitly correlated methodologies, or of composite schemes where we combine DFT/MP2 methods with either standard or explicitly correlated techniques, or of SAPT based methods, and of machine learning techniques. Several examples will be used presented and discussed.

Dr. Matteo Gori

Leveraging the Many-Body Dispersion Model: Accessing Charge Density Distortions and Quantum Electrodynamics Properties in Large Molecular Systems

15:30 - 16:10

Department of Physics and Materials Science, University of Luxembourg, Luxembourg City, Luxembourg

The Many-Body Dispersion (MBD) model is a highly accurate and effective approach for describing many-body van der Waals interactions in post-DFT calculations. Unlike other methods with similar goals, the MBD model characterizes the electronic response properties of the charge density field using a set of quantum Drude oscillators—quantum harmonic oscillators that carry an electric dipole. This representation has the potential to capture additional aspects of the electronic structure beyond many-body dispersion energy corrections, particularly in large molecular systems such as realistic biomolecular complexes. Motivated by this picture, we present a twofold investigation into the capabilities of the MBD model for describing the geometry of electronic quantum charge distributions and localized (paramagnetic) currents in large molecular systems. First, we demonstrate how the MBD model can be employed to capture distortion effects on the ground-state charge density induced by many-body dispersion interactions, with potential applications in density-corrected DFT and in the visualization of dispersion interactions within large molecules. Second, we explore how the MBD model can be embedded within the established molecular Quantum Electrodynamics (QED) framework, offering an effective representation of the polarization and magnetization field operators in large molecular systems. This integration opens new avenues for applications such as polariton chemistry in QED cavities and chiral discrimination interactions in biomolecular systems.

Prof. Cina Foroutan-Nejad

Collective Interactions

Institute of Organic Chemistry, Polish Academy of Science, Warsaw, Poland

16:10 - 16:30

A century after G. N. Lewis introduced his foundational model of chemical bonding, its core principles remain central to our understanding of molecular structure. Traditionally, neighboring atoms in a Lewis structure are assumed to share stabilizing interactions. However, this assumption begins to falter at the boundary between covalent and noncovalent bonding. Our work reveals that, in certain molecules with the general formula MAX—where M is a metal, A a nonmetal, and X an electron-rich or electron-withdrawing group—the interaction between adjacent M and A atoms can be destabilizing. Remarkably, the overall structure is preserved due to strong interactions between electron-deficient metals and the X groups.[1–6] This phenomenon gives rise to unconventional structures, such as the inverted LiCF, where lithium interacts preferentially with fluorine atoms over the central carbon in the gas phase. These collective interactions extend beyond organometallic compounds and offer insight into anomalous bond dissociation energies and stability trends across a wide range of molecules—from perhaloalkanes to the elusive cyclic CO. Our computational studies highlight the broad relevance of this concept in modern chemical bonding theory.

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Prof. Katherine Hunt

Charge densities and London dispersion forces

Department of Chemistry, Michigan State University, East Lansing, Michigan, USA

16:30 - 17:10

In 1939, Feynman published without proof a statement that the dispersion force between two atoms in S states comes from the attraction of each nucleus to the distorted electronic charge distribution in its own vicinity. In 1990, Hunt proved Feynman's statement by use of perturbation theory within the polarization approximation and extended the result to molecules of arbitrary symmetry. Later work has raised question about this interpretation. In 2019, Kooi and Gori-Giorgi developed a density-functional theory that yields the dispersion energy with high accuracy, with no change in the electronic charge density at any order. Calculations on He and Ar atom pairs show that the electron density drops in the immediate vicinity of each nucleus, within the van der Waals bonding region. My group has derived dispersion forces with high accuracy from the correlation contribution to the charge density of the hydrogen molecule in the lowest triplet state at long range. As found previously, the electron density drops in the immediate vicinity of each nucleus, within the bonding region. However, the electron density that produces the forces on the nuclei rises in the same region, validating Feynman's statement.

Day 3 | Morning Presentations. Chair: Dr. Ariadni Boziki

October 17th, 9:00 – 12:00 CET

Prof. Ganna Gryn'ova

Engineering Functional Organic Materials through Noncovalent Interactions

09:00 - 09:40

Gregor Lauter[1], Catherine Mollart[1], Michelle Ernst[2] and Ganna Gryn'ova[1, 2]
[1]School of Chemistry, University of Birmingham, B15 2TT Birmingham, United Kingdom
[2]Institute for Geological Sciences, University of Bern, 3012 Bern, Switzerland

Functional, topologically complex organic systems are rising stars in modern materials science due to their biocompatibility, structural variability, and wealth of physico-chemical properties. Their practical applications often involve interactions with small molecular targets (e.g., gases, environmental pollutants, and drugs) via relatively weak non-covalent forces. In this contribution we will discuss our recent efforts towards reliable yet scalable computational approaches to modelling, quantifying, and analysing the interactions between functional organic materials and their small molecule targets. We focus on two types of systems: (1) graphene-based materials for sensing and catalysis, and (2) organic frameworks for molecular storage. We will highlight the methodological tips and tricks for modelling the relevant host-guest complexes using multiscale approaches at an optimal ratio of accuracy and computational cost and illustrate how intermolecular forces can guide targeted design of novel catalysts and cages.

Prof. Christoph Bannwarth

Non-covalent interactions in molecular photocatalysis and photophysics

09:40 - 10:20

Institute of Physical Chemistry, RWTH Aachen University, Aachen, Germany

The ability to predict optical molecular properties and photochemical reaction outcomes using quantum chemistry methods becomes increasingly important for improving our mechanistic understanding and for advancing the computer-aided design of molecular emitters and photocatalysts. Key is the proper simulation of the photoinduced decay processes in the condensed phase. In photocatalysis, the reaction pathways not only depend on the involved excited states, but also on the formation of a non-covalent complexes between the photocatalyst and the substrate. We will discuss a recently investigated photocatalytic cleavage reaction of chiral oxetanes. [1] Different cleavage pathways were found and shown to be dependent on the formation of stable non-covalent complexes between the catalyst and the substrate. Furthermore, the enantioselectivity can be rationalized from different association constants with the photocatalyst, the competition with cleavage products, and the substrate self-association. Additionally, we will discuss the influence of excimer formation on the photoluminescence quantum yields (PLQYs) of luminescent organic molecules. Particularly, the formation of charge transfer states in these complexes can lead to significant reduction of the PLQY.[2] We show that these processes can be modeled quite well using state-specifc orbital optimized density functional theory methods with dispersion corrections.

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Dr. Dzmitry Firaha

Neumann-Perrin dispersion correction. Twenty years of application in molecular crystal modelling

10:40 - 11:20

Dzmitry Firaha, Subhayan Roychoudhury, Marcus Neumann
Avant-garde Materials Simulation, Merzhausen, Germany

Accurate modelling of van der Waals interactions is essential for predicting the structure and stability of molecular crystals. The Neumann-Perrin (NP) dispersion correction [1], which is ne of the first physically grounded empirical based dispersion correction to the density functional theory, celebrates its 20 year anniversary this year. Originally parametrized in 2005, this correction has demonstrated robust performance for industrial crystal structure prediction (CSP) problems over the past two decades[2]. A key strength of the NP approach lies in its consistent reproduction of experimental crystal structures[3], which is an essential prerequisite for success in blind test CSP challenges[4]. The structures obtained with the NP correction have been used to calculate reliable and accurate free energies with TRHu(ST)23 method[5] to predict the stability of crystal forms under varying temperature and humidity conditions (Fig. 1). Our predictions align closely with experimental stability data, phase-transition temperatures and phase-transition relative humidities, highlighting the usefulness of these calculations to guide experimental screening and drug-formulation strategies.
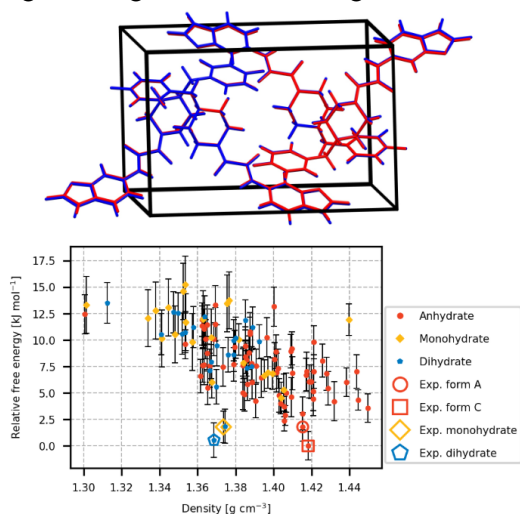

Figure 1. On the left is an overlay of an experimental structure in red and the PBE-NP energy minimized structure in blue of radiprodil form A. On the right is a free-energy landscape of radiprodil hydrate and anhydrate forms at 298.15 K and a relative humidity of 50

We demonstrate that the NP correction yields excellent agreement with experimentally determined lattice parameters and molecular arrangements across a broad range of organic crystals and compare it with other dispersion corrections models available to the community. These results underline the enduring value of the NP correction in bridging the gap between first-principles modelling and experimental crystallography, and in enabling in silico materials design starting from accurate dispersion modelling.

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2) Neumann, M. A., et al. (2015), Nature Comm., 6.1, 7793; Hoja, J., et al. (2019), Sci. Adv. 5.1, eaau3338.
3) van de Streek, J., Neumann, M. A. (2010), Struct. Sci., 66.5, 544; van de Streek, J., Neumann, M. A. (2014), Struct. Sci., 70.6, 1020.
4) Day, G. M., et al. (2009). Struct. Sci., 65.2, 107; Bardwell, D. A., et al. (2011). Struct. Sci., 67.6, 535; Reilly, A. M., et al. (2016). Struct. Sci., 72.4, 439; Hunnisett, L. et al. (2024). Acta Cryst. B80, 517; Hunnisett, L. et al. (2024). Acta Cryst. B80, 548.
5) Firaha, D. et al. (2023). Nature 623, 324.

Dr. Johannes Hoja

Anharmonic Intermolecular Vibrations of Molecular Crystals via Vibrational Perturbation Theory

11:20 - 11:40

Department of Chemistry, University of Graz, Graz, Austria

Low-frequency vibrations of molecular crystals are extremely challenging to describe, but are the most crucial part for determining vibrational entropy and hence free energies at finite temperatures, often leading to qualitative changes in the stability ordering of polymorphs [1]. Furthermore, THz spectroscopy enables the distinction between such different crystal-packing arrangements of the same molecule. These low-frequency vibrations are collective lattice modes representing intermolecular translations and rotations and are often dominated by van der Waals dispersion interactions. Therefore, an accurate account of dispersion interactions in the utilized electronic structure method is essential. In terms of the vibrational description, the harmonic or quasi-harmonic approximation is often insufficient given the anharmonic nature of many intermolecular modes. We have recently shown that a very good description of experimental fundamental frequencies, within about 6 cm-1 on average, can be obtained for molecular dimers by using second-order vibrational perturbation theory (VPT2) combined with hindered-rotor models together with CCSD(T) calculations [2]. Herein, we introduce a VPT2 approach that can be applied to periodic molecular crystal structures. Anharmonic force constants are calculated for monomers and relevant dimers of the respective crystal, which are then embedded into fully periodic harmonic calculations using a multimer embedding scheme [3]. We illustrate this approach for small dispersion-bound molecular crystals evaluated at the PBE+MBD level with a special focus on the accuracy of low-frequency intermolecular vibrations. This approach also yields improved free energies that are vital for calculating lattice energies or energy barriers for transformations between molecular crystal polymorphs [4], for which dispersion interactions play an imperative role as well. Compared with canonical fully periodic VPT2 calculations, the introduced fragment approach is far more cost-effective and paves the way toward highly accurate predictions of THz spectra and vibrational free energies for molecular crystals.

1) J. Hoja, H.-Y. Ko, M. A. Neumann, R. Car, R. A. DiStasio Jr., A. Tkatchenko, Sci. Adv. 5, aau3338 (2019).
2) J. Hoja, A. D. Boese, J. Chem. Phys. 161, 234110 (2024).
3) J. Hoja, A. List, A. D. Boese, J. Chem. Theory Comput. 20, 357–367 (2024).
4) N. Goncharova, J. Hoja, arXiv preprint, arXiv:2410.10506 (2025).

Bastien Courbiere

**Chemical reactivity from a combined Conceptual DFT and ELF topology approach**

11:40 - 12:00

B. Courbière, J. Pilmé
Laboratoire de Chimie Théorique, Sorbonne Université, Paris 75005, France

Unravelling chemical reactivity can be compared to solving a puzzle: understanding how molecules interact, reorganize, and evolve during a reaction requires both empirical insight and intuition. The study of reactivity, developed to assist experimentalists and provide rationalization tools, is a well-established field in molecular modelling. However, most approaches rely on computationally demanding methods or require long calculation times. This project introduces an innovative method to predict the energetic profile of chemical reactivity, from separated reactants to transition states, at a low computational cost. By combining the Dual Descriptor (DD)[1], from Conceptual DFT[2-3], condensed within the Electron Localization Function (ELF)[4] topology, we propose an approach that captures early-stage interactions while mimicking the DFT energies. Our approach builds on the Klopman-Salem[5-6] model, which isolates Coulomb contributions between molecular fragments treated as monomers. The so-called "EDD", depends entirely on the relative orientation between the "frontier" densities of molecular fragments. By integrating ELF probability indicators within Dual Descriptor domains, this framework[8] offers a fast, cost-effective and computationally accessible alternative to traditional methods, providing a reliable and efficient way to understand and predict chemical reactivity. We illustrate this approach on several prototypical reactions, from simple non-covalent interactions to intricate reactivity profiles.

1) C. Morell, A. Grand, A. Toro-Labbé, New Dual Descriptor for Chemical Reactivity, J. Phys. Chem. A 109, 205–212 (2005)
2) W. Yang, R. G. Parr, Hardness, Softness, and the Fukui Function in the Electronic Theory of Metals and Catalysis, Proc. Natl. Acad. Sci. U. S. A. 82, 6723–6726 (1985)
3) R. G. Parr, W. Yang, Density-Functional Theory of the Electronic Structure of Molecules, Annu. Rev. Phys. Chem. 46, 701–728 (1995)
4) B. Silvi, A. Savin, Classification of Chemical Bonds Based on Topological Analysis of Electron Localization Functions, Nature 371, 683–686 (1994)
5) L. Salem, Intermolecular Orbital Theory of the Interaction between Conjugated Systems. I. General Theory, J. Am. Chem. Soc. 90, 543–552 (1968)
6) G. Klopman, Chemical Reactivity and the Concept of Charge- and Frontier-Controlled Reactions, J. Am. Chem. Soc. 90, 223–234 (1968)
7) J. Klein, P. Fleurat-Lessard, J. Pilmé, New Insights in Chemical Reactivity from Quantum Chemical Topology, J. Comput. Chem. 42, 840–854 (2021)
8) B. Courbière, J. Pilmé, Exploring Chemical Reactivity through a Combined Conceptual DFT and ELF Topology Approach, J. Mol. Model. 30, 362 (2024)
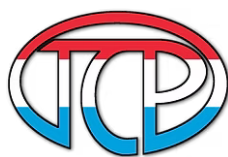
Day 3 | Afternoon Presentations. Chair: Dr. Matteo Gori

October 17th, 13:50 – 16:50 CET

Prof. Xiaofei Liu

Van der Waals Force and Torque—Macroscopic and Microscopic Descriptions

State Key Laboratory of Mechanics and Control for Aerospace Structures, Key Laboratory for Intelligent Nano Materials and Devices of the Ministry of Education, Nanjing University of Aeronautics and Astronautics, Nanjing, China

Van der Waals (vdW) interaction can be described either by microscopic theories such as ab initio quantum mechanical method and force-filed approximation or by macroscopic theories such as Lifshitz theory. It is highly desirable to achieve consistencies between the atomistic and continuum theories. Recent years, we revealed the dielectric function effect on the interlayer interaction of 2D materials and the vdW screening effect by graphene, by both theoretical and experimental investigations. Fifty years after the prediction of dielectric anisotropy-induced vdW torque by Parsegian et al., the effect can only be described by the continuum theory till now. We recently reproduced the vdW torque between dielectrically anisotropic 2D materials and related torque scaling laws using the fully atomistic many-body dispersion model. Also, we demonstrate a molecular simulation-compatible pairwise approximation that results in a dielectric function criterion of sign of vdW force formally identical to the Lifshitz criterion. Namely, the force computed from interatomic energy sum with materials' and liquid's C6 coefficients derived from Clausius-Mossotti relation will be repulsive, if liquid's dielectric function ranks in-between those of unlike interacting materials.

13:50 - 14:30

Dr. Prokop Hapala

Grid-projected force-fields for high throughput simulations of molecules on surface

14:30 - 14:50

Prokop Hapala (FZU - Institute of Physics of the Czech Academy of Sciences, Na Slovance 1999/2, Prague 8, 182 00, Czech Republic),
Paolo Nicolini (FZU - Institute of Physics of the Czech Academy of Sciences, Na Slovance 1999/2, Prague 8, 182 00, Czech Republic),
Indranil Mal (FZU - Institute of Physics of the Czech Academy of Sciences, Na Slovance 1999/2, Prague 8, 182 00, Czech Republic),
Milan Kocí (FZU - Institute of Physics of the Czech Academy of Sciences, Na Slovance 1999/2, Prague 8, 182 00, Czech Republic),
Niko Oinonen (Aalto University, Department of Applied Physics, P.O. Box 11000, Otakaari 1B, AALTO, FI-00076, Finland),
Aliaksandr V. Yakutovich (nanotech@surfaces laboratory, Swiss Federal Laboratories for Materials Science and Technology, Empa, Überlandstrasse 129, Dübendorf, CH-8600, Switzerland),
Aurelio Gallardo (IMDEA Nanoscience Institute, C/ Faraday 9, Campus de Cantoblanco, Madrid, 28049, Spain),
Martin Ondráček (FZU - Institute of Physics of the Czech Academy of Sciences, Na Slovance 1999/2, Prague 8, 182 00, Czech Republic),
Ondřej Krejčí (Aalto University, Department of Applied Physics, P.O. Box 11000 (Otakaari 1B), AALTO, FI-00076, Finland)

Rapid exploration of molecular configurations on surfaces is crucial for the design and rationalization of self-assembled structures, as well as for simulations of molecular manipulation using scanning probe microscopy - both essential for advancing molecular electronics and nanotechnology. The computational bottleneck in these simulations typically lies in evaluating non-covalent interactions between molecules and substrates, even when using simple pairwise potentials such as Lennard-Jones or Morse. To address this challenge, we developed the Grid-Projected Force Field (GridFF) method, which leverages the rigidity of the substrate by replacing explicit pairwise non-covalent interactions between atoms with interpolation from a precomputed grid. This not only accelerates simulations by 1–2 orders of magnitude but also enables the use of more sophisticated interaction potentials at virtually no additional computational cost. We have implemented GridFF in two high-throughput simulation packages. The first, ppafm [1], simulates 3D stacks of high-resolution atomic force microscopy (AFM) images (1 million pixels) in less than 0.1 seconds, with accuracy comparable to density functional theory (DFT). This is achieved using GridFF constructed from convolution of ab initio electron densities and Grimme D3 van der Waals corrections. The ppafm package has become a primary tool for generating training data for machine-learning-based reconstruction of molecular structures from AFM images [2]. The second application is FireCore [3], a newly developed package for configuration sampling of small organic molecules on surfaces. FireCore exploits GPU parallelism to run thousands of system replicas simultaneously, enabling the sampling of 15 million configurations per second of a xylitol molecule on a NaCl substrate using a single desktop GPU. We envision FireCore playing a role in training autonomous nanomanipulation protocols analogous to the role ppafm plays in imaging. To further enhance the accuracy of these simulations, we are currently integrating efficient hydrogen-bond corrections into the GridFF framework.

1) Oinonen, N. et al. Advancing scanning probe microscopy simulations: A decade of development in probe-particle models. Computer Physics Communications 305, 109341 (2024).
2) Alldritt, B. et al. Automated structure discovery in atomic force microscopy. Sci. Adv. 6, (2020).
3) https://github.com/ProkopHapala/FireCore

Dr. Ariadni Boziki

The role of van der Waals interactions on the response properties of materials

Department of Physics and Materials Science, University of Luxembourg, Luxembourg City, Luxembourg

The accurate modeling of materials requires a careful treatment of van der Waals (vdW) interactions, which govern not only structural organization but also dynamic response properties. In this talk, I will examine how vibrational spectra and related observables in molecular crystals are shaped by dispersion forces, and how different theoretical models; including pairwise and many-body vdW corrections affect the predicted behavior. By systematically comparing results obtained with different dispersion-inclusive functionals, I will highlight the strengths and limitations of these methods in accurately capturing experimental observables. This discussion aims to underscore the necessity of an accurate treatment of vdW forces in modeling complex materials and guiding the design of new solids.

14:50 - 15:30

Gianluca Regni

ADLD and ADEX: New Lenses for Atomic-Level Analysis of Non-Covalent Interactions

University of Perugia, Perugia, Italy

We present a novel quantum chemical method for quantifying atomic contributions to London dispersion (LD) energy in molecular systems, with a "gold standard" accuracy within the Local Energy Decomposition framework. This method, called Atomic Decomposition of London Dispersion energy (ADLD), decomposes LD interactions into atom-wise contributions, providing a clearer and more interpretable picture of how dispersion affects each part of the molecule. This level of resolution is especially powerful for large and complex systems, where it is often difficult to intuitively identify which functional groups contribute most to the total dispersion energy. ADLD also makes it possible to observe how London dispersion responds to variations in electronic structure, such as spin state, charge, and resonance, directly at the atomic level, offering valuable insights for molecular design in both drug discovery and materials science. In addition to ADLD, we also present the Atomic Decomposition of EXchange energy (ADEX) method, which provides an analogous atom-wise partitioning for the exchange energy within the LED framework. Together, ADLD and ADEX help provide atom-wise insights into key components of non-covalent interactions within molecular systems, enhancing our ability to analyze and design complex molecules.
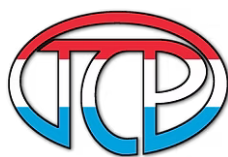
15:50 - 16:10

Prof. Mariana Rossi

Unraveling the Nuclear Motion of Weakly Bound Materials   **16:10 - 16:50**

MPI for the Structure and Dynamics of Matter, Hamburg, Germany

Weakly bonded interfaces composed by molecular and solid-state inorganic materials give rise to a rich variety of nuclear motion and tunable nuclear structure that is tightly connected to diverse electronic properties in these systems. In my talk, I will discuss the importance of accounting for nuclear motion to study diverse properties of these systems, and the importance of doing so. I will show how we push the limits of density-functional theory and different ab initio techniques that capture nuclear motion to unravel the properties of realistic interfaces [1]. I will discuss how they can be connected to first-principles electronic structure and machine-learning approaches [2,3]. Applications where the quantum nature of the nuclei become indispensable to assess structural and electronic properties these interfaces will be shown and discussed [4], as well as how these can be characterised by the simulation of experimentally observable quantities like tunneling rate constants and advanced vibrational spectroscopy [5,6].

1) J. Chem. Phys. 154, 170902 (2021);
2) J. Chem. Theory Comput. 17, 7203- 7214 (2021);
3) J. Chem. Phys. 159, 014103 (2023);
4) arXiv:2411.10994 (2024)
5) J. Chem. Phys. 156, 194106 (2022);
6) J. Phys. Chem. Lett. 14, 6850 (2023)

Organisers

Prof. Dr. Alexandre Tkatchenko
Université de Luxembourg

Prof. Dr. Jean-Pierre Djukic
Université de Strasbourg

Mirela Puleva
Université de Luxembourg

Sergio Suárez Dou
Université de Luxembourg