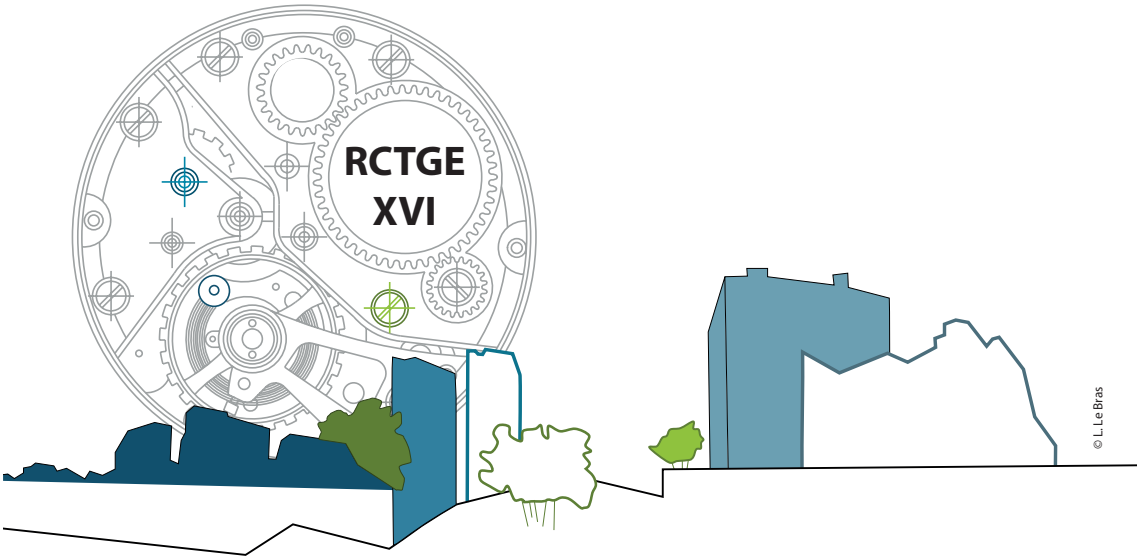


Rencontres des Chimistes Théoriciens du Grand Est

2 et 3 juillet 2025

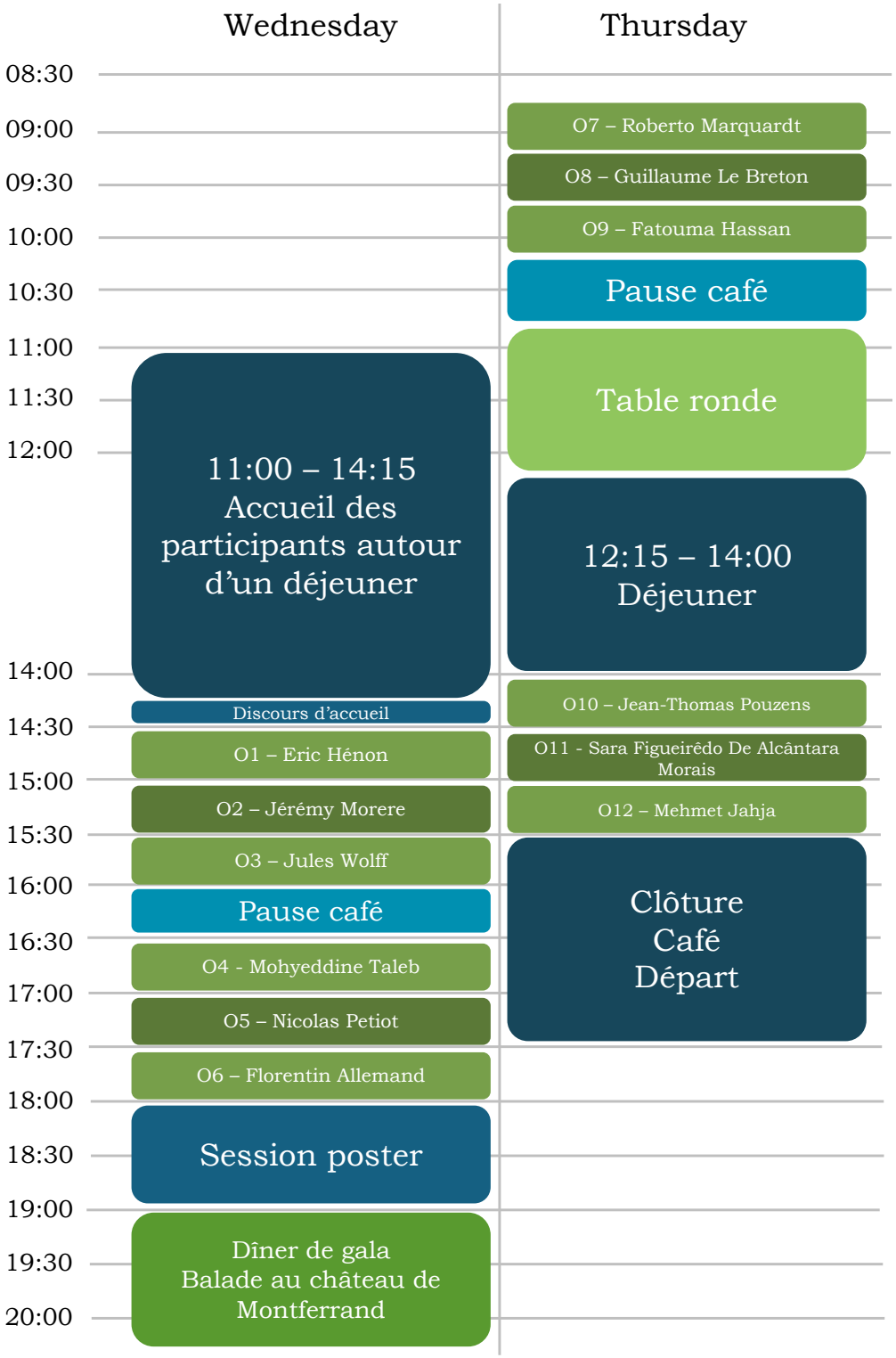
ABSTRACT BOOKLET

Table of Contents

List of participants

NOM	Prénom	Etablissement
ALLEMAND	Florentin	Ecole Polytechnique
AMINI VALASHNI	Mohammad	Université de Strasbourg
BIGNON	Emmanuelle	Université de Lorraine
BIN JASSAR	Mohammed	Ecole Normale Supérieure, Université PSL
BRUNETTI	Filippo	Université de Lorraine
CARDEY	Bruno	Université Marie et Louis Pasteur
CAROF	Antoine	Université de Lorraine
CHAPUIS	Simon	Université de Strasbourg
CHAUMONT	Alain	Université de Strasbourg
CORNATON	Yann	Université de Strasbourg
DUMA	Luminita	Université de Reims Champagne-Ardenne
ETIENNE	Thibaud	Université de Lorraine
FIGUEIRÊDO DE ALCÂNTARA MORAIS	Sara	Université de Strasbourg
HASSAN MOUSSA	Fatouma	Université Marie et Louis Pasteur
HENON	Eric	Université de Reims Champagne-Ardenne
JAHJA	Mehmet	Université Bourgogne Europe
KHARTABIL	Hassan	Université de Reims Champagne-Ardenne
LE BRAS	Laura	Université Marie et Louis Pasteur
LE BRETON	Guillaume	Université Bourgogne Europe
LESNICKI	Dominika	Université de Lorraine
LOIR-MONGAZON	Lucas	Université de Strasbourg
MORERE	Jérémy	Université de Lorraine
PASTORE	Mariachiara	Université de Lorraine
PETIOT	Nicolas	Université Bourgogne Europe
POUZENS	Jean-Thomas	Université Bourgogne Europe
RANDRIHARIMANAMIZARA	Ulrick Fineddie	Université Bourgogne Europe
TALEB	Mohyeddine	Université de Reims Champagne-Ardenne
WILLIG	Charles	Université de Lorraine
WOLFF	Jules	Université de Strasbourg

Program


Wednesday
Thursday
08:30
09:00
09:30
10:00
10:30
11:00
11:30
12:00
14:00
14:30
15:00
15:30
16:00
16:30
17:00
17:30
18:00
18:30
19:00
19:30
20:00
O7 – Roberto Marquardt
O8 – Guillaume Le Breton
O9 – Fatouma Hassan
Pause café
Table ronde
11:00 – 14:15
Accueil des participants autour d'un déjeuner
12:15 – 14:00
Déjeuner
Discours d'accueil
O1 – Eric Hénon
O2 – Jérémy Morere
O3 – Jules Wolff
Pause café
O4 - Mohyeddine Taleb
O5 – Nicolas Petiot
O6 – Florentin Allemand
Session poster
Dîner de gala
Balade au château de Montferrand
O10 – Jean-Thomas Pouzens
O11 - Sara Figueirêdo De Alcântara Morais
O12 – Mehmet Jahja
Clôture
Café
Départ

Oral Communications

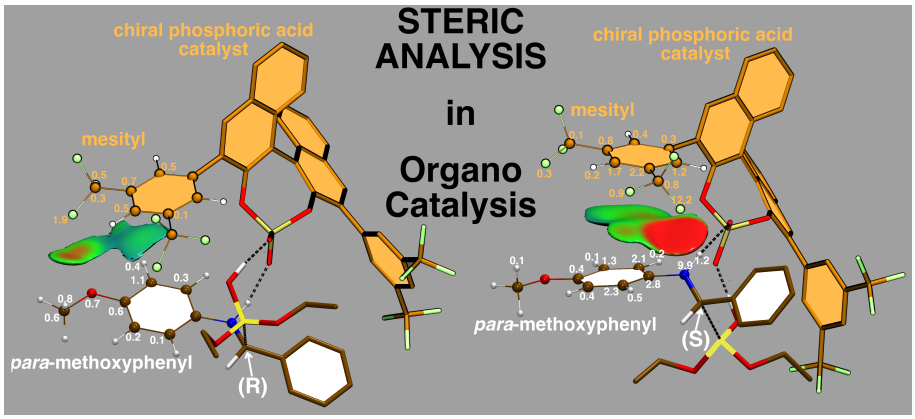
O1 - A Practicable Measure and Spatial Vizualisation of Steric repulsion with Atomic Resolution

Eric Hénon*[1]
[1] Institut de Chimie Moléculaire de Reims, UMR CNRS 7312, Université de Reims Champagne-Ardenne, Moulin de la Housse, Reims, France

Steric repulsion, often regarded as a macroscopic manifestation of the Pauli exclusion principle, challenges previous assumptions in organic chemistry, transition metal and non-covalent chemistry.[(1,2)] While its importance is widely recognized, visualizing where and how it occurs remains challenging. Tools like SAPT[(3)] exist for assessing Pauli repulsion, but they condense the characteristics of this repulsion into a single number. We present the **Steric Effect Localization Function** (**SELF**, soon in the program IGMPlot, http://igmplot.univ-reims.fr), a novel approach providing:

1. Three-dimensional visualization of steric interactions
2. Quantification of local steric repulsion and integration
3. Atomic-level decomposition of Pauli effects

The method builds on the core concept underlying the Electron Localization Function (ELF), namely, the kinetic energy excess (KEE) due to the Pauli exclusion principle. The key innovation lies in decomposing the Pauli KEE density into inter- and intra-fragment contributions, with the inter-fragment term directly mapping steric interactions. By integrating this with the Independent Gradient Model (IGM),[(4)] SELF delivers unparalleled insights into where steric interactions occur and which atoms contribute most significantly (see the illustrative example on the figure).



SELF is grounded in quantum mechanical principles, providing a physically sound basis for steric analysis. We validated **SELF** across diverse chemical scenarios, including:

- Atropoisomerism dynamics, revealing the evolution of atomic contributions during hindered rotation
- Organo-catalyzed reactions, showing how steric interactions govern transition state stereoselectivity

SELF approach enables user-friendly atom-resolved visualization and quantification of steric effects, offering both interpretative clarity and computational rigor, complementing existing computational methods.

(1) T. A. Hamlin, F. M. Bickelhaupt, I. Fernández, *Acc. Chem. Res.*,**2021**, 54, 8, 1972-1981
(2) L. Hu, H. Gao, Y. Hu, Y.-B. Wu, X. Lv, G. Lu, *J. Org. Chem.*, **2023**, 88, 2750-2757
(3) B. Jeziorski, R. Moszynski, K. Szalewicz, *Chem. Rev.*, *1994*, 94, 1887-1930
(4) a) C. Lefebvre, G. Rubez, H. Khartabil, J.-C. Boisson, J. Contreras-García, E. Hénon, *Phys. Chem. Chem. Phys.*, **2017**, 19, 17928-17936 b) C. Lefebvre, J. Klein, H. Khartabil, J.-C. Boisson, E. Hénon, *J. Comp. Chem.*, *2023*, 44, 1750-1766

O2 - Catalan numbers, Dyck language, and second quantization: An algorithm-oriented representation of second quantization chains

Jérémy Morere*[1] and Thibaud Etienne[1]
[1]Laboratoire de Physique et Chimie Théoriques - CNRS and Université de Lorraine

Second quantization is a fundamental formalism in quantum chemistry and condensed matter physics for describing systems of bosonic and fermionic particles. For electrons, this formalism enables the systematic manipulation of Slater determinants and operators representing observables, based on the anti-commutation and hermiticity rules of creation and annihilation operators. Second quantization operators are used in methods to describe many-body systems, such as coupled-cluster theory or configuration interaction.
Evaluating the expectation value of a chain of second quantization operators is a central challenge. Wick's theorem makes it possible to simplify the evaluation of an expectation value of a chain, relative to a vacuum, by expressing it as the normal order of the chain plus a sum of all contractions of the chain taken in normal order. That expectation value, with respect to the physical or Fermi vacuum, is given by the sum of the expectation values of the fully contracted terms. In fact, the expectation value of any non-fully contracted term is zero. The main advantage of this formulation is that it reduces the problem to finding all fully contracted terms. These terms can be expressed in terms of products of Kronecker deltas. In other words, finding the expectation value becomes a problem of finding viable pairings of second quantization operators. If this procedure is well defined, the number of terms generated by the contractions grows rapidly, making the computations costly in terms of time and memory. In addition, a significant number of the fully contracted terms will be zero, so it seems necessary to find criteria to limit the calculations to the non-zero terms as much as possible.
In this talk we propose a translation of chains of second quantization operators into a Dyck language. A word in a Dyck language can be seen as a string of left and right parenthesis (and/or brackets). If a word corresponds to a balanced string, it is called a Dyck word. In a chain of second quantization operators, each operator is translated into left or right parenthesis. If the resulting string is a Dyck word, the expectation value of the chain is non-zero. Two examples are given below. Let $|\rangle$ denote the physical vacuum:

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

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

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

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

is a non-zero while

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

is zero. However, after translation, it is clear that the first string is balanced and the second is not, implying the nullity of the second expectation value. The enumeration of chains of operators with a non-zero expectation value then joins the large family of problems for which Catalan numbers are the solution. This family includes Dyck language, triangulation of polygons, or some graph problems. This analogy makes it possible to formulate non-nullity rules for the expectation value of chains of operators. At the same time, tools used to describe Dyck words, can be used to predict the number of non-zero terms in the sum after applying Wick's theorem. A similar relationship can be made with respect to the Fermi vacuum, allowing us to work with Slater determinants.
The graphical representation of admissible chains has enabled us to develop an algorithm for symbolically evaluating the expectation value of a 1-body operator between two Slater determinants. The strength of this algorithm is to reduce as much as possible the number of second quantization operator pairings to be taken into account to obtain the result, thus reducing the complexity of the algorithm.

(1) T. Etienne, *arxiv repository*, 1811.08849v15, sec. 5.2, **2018**

O3 - Cations Effect on Pt Electrodes in Alkaline HER Conditions Studied by Molecular Dynamics at Constant Potentials

Jules Wolff*[1,2], Laurent Ruhlmann[2], Antoine Bonnefont[3], Alain Chaumont[4], and Tristan Asset[1],
[1] ICPEES, CNRS-ECPM-Université de Strasbourg, 67087, Strasbourg Cedex 2, France
[2] Institut de Chimie, CNRS-Université de Strasbourg, 67000, Strasbourg, France
[3] University Grenoble Alpes, University of Savoie Mont Blanc, LEPMI, 38000 Grenoble, France
[4] Chimie de la Matière Complexe, Faculté de Chimie, 67081 Strasbourg Cedex, France

Rising interest for dihydrogen as an energy vector has been putting the hydrogen evolution reaction (HER) at the forefront of research. The HER has been highly studied and optimized at different scales: catalyst design, operating conditions (pH, temperature) and electrolyte. At the electrolyte level, the crucial role of the cations has been highlighted on Pt, hinting that their re-organization within the electrochemical double layer (EDL) may critically influence a given reaction kinetics(1). A coherent mapping of the EDL structure can be obtained using molecular dynamics (MD) in order to rationalize this influence. In 2020, the MetalWalls package was developed in order to perform 'all atoms constant potential MD' and has been enabling a detailed mapping of the EDL(2). With the aim of unveiling the link between cations nature and the electrode/electrolyte properties, this study focuses on MD simulations at 0 and 1V on platinum monocrystalline facets. Different electrolytes (1M NaOH, KOH, CsOH) are investigated. Key properties such as solvation, cation and water distribution or water orientation are obtained, as illustrated in Figure 1, and the pivotal influence of the cation nature on these properties evidenced. The observed properties are then discussed in the light of experimental observations to correlate electrode/electrolyte interface properties and HER activity(3).

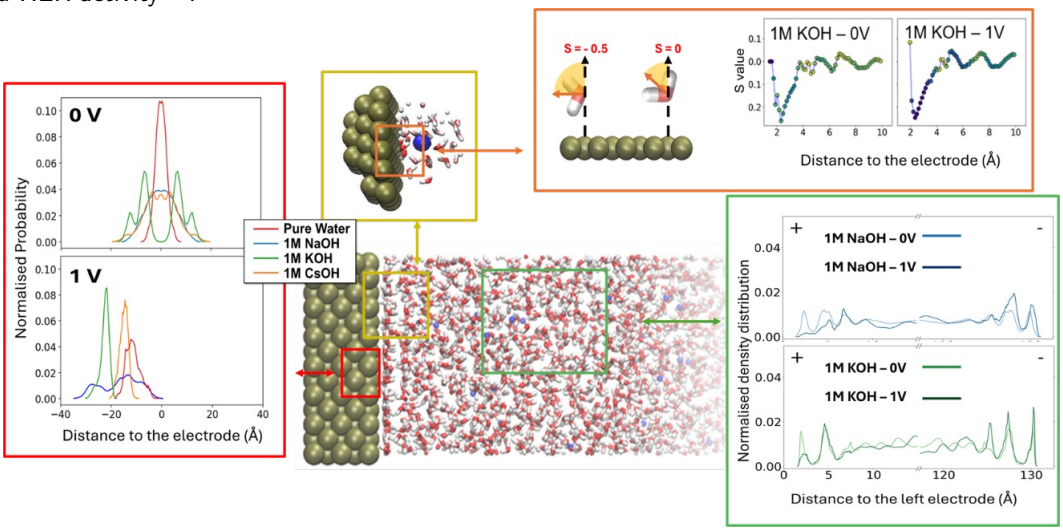


Figure 1: Visual representation by Visual Molecular Dynamics (VMD) of a 1M NaOH system. Extracted data are presented as electrode charge for system with different cation types (red box), view of a solvated Na+ near Pt(100) electrode (yellow box), orientation of water near the electrode measured through the orientation order parameters for K+ systems (orange box), density profile of Na+, and K+ along the z axes of the box (green box). The simulation were performed at 0 and 1V during 20-30 ns in a box of 14nm long.

(1) M. M. Waegele *et al.*, *J. Chem. Phys.*, **2019**, 151, 160902
(2) A. Marin-Laflèche *et al.*, *J. Open Source Softw.*, **2020**, 5(53), 2373
(3) A. Goyal *et al.*, *J. Am. Chem. Soc.*, **2024**, 146, 7305-7312

O4 - In-silico exploration of BcTSPO: protein-ligand interactions probed by docking and dynamics simulations

Mohyeddine Taleb*[1], Julien Diharce[2], Catherine Etchebest[2], Éric Hénon[1], Jean Jacques Lacapère[3], Luminita Duma[1]
[1] University of Reims Champagne-Ardenne, CNRS, ICMR UMR 7312, 51687 Reims, France
[2] Université Paris Cité and Université de la Réunion, BIGR laboratory, DSIMB, UMR S1134, 8 Rue Maria Helena Vieira Da Silva, 75014 Paris, France
[3] Sorbonne Université, Ecole normale supérieure, PSL University, CNRS, Laboratoire des Biomolécules, LBM, 75005 Paris, France

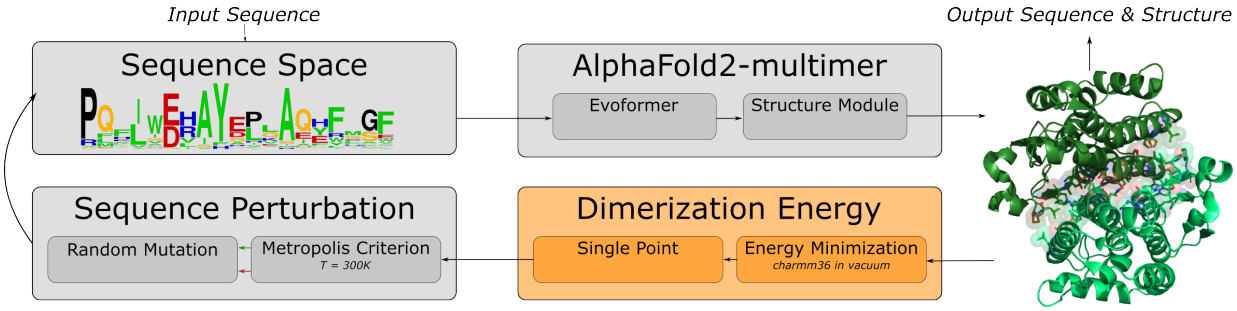
The 18 kDa Translocator Protein (TSPO), a highly conserved transmembrane protein primarily located in the outer mitochondrial membrane(1), is recognized as a multifunctional biomarker and pharmacological target in neurodegenerative and inflammatory diseases(2). Although structural studies have characterized mammalian and bacterial TSPO(3–5), the molecular basis of ligand binding, particularly in bacterial homologs remains poorly understood. In this study, we employed a comprehensive computational approach to investigate ligand interactions with Bacillus cereus TSPO (BcTSPO, PDB: 4RYI). We evaluated the binding of five relevant ligands - PK 11195, diazepam, Ro5-4864, HEME, and protoporphyrin IX (PPIX) - using AutoDock molecular docking. IGMPlot protomolecular electron density (Dg, a measure of electron density within the binding cavity)(6) was used to quantify the contribution of amino acids within the binding cavity. Subsequent Gromacs molecular dynamics simulations in a DOPC membrane environment, including ions and water molecules, assessed the conformational dynamics of the X-ray BcTSPO structure, in the absence of the ligand (apo form). Clustering of 3 apo trajectories (1 μs each) and principal Component Analysis revealed seven representative conformations. To explore the impact of protein flexibility on ligand binding, **each of these conformations was subsequently used in independent docking experiments against the five ligands**, to evaluate the impact of protein dynamics on ligand binding.
The stability of the re-docked structures was assessed by performing a 100 ns molecular dynamics simulation, MMPBSA, IGMPlot protomolecular electron densities (Dg) and RMSD were performed. The results show the Porphyrin-based ligands (HEME and PPIX) demonstrated the highest binding affinities using MMPBSA (kcal/mol) and IGMPlot (Dg), particularly in conformational states with large binding cavities. This study highlights the dynamic nature of BcTSPO like experimentally observed for the mouse TSPO in proteoliposomes(7). Our finding demonstrates the role of ligand flexibility, cavity adaptability, and π-π stacking interactions in stabilizing TSPO-ligand complexes.
The computational prediction of binding affinities and the molecular-level binding modes provide insights into the structural and energetic landscapes of BcTSPO-ligand interactions, offering a valuable foundation for future experimental studies in different membrane mimetic environments.

(1) V. Papadopoulos *et al.*, *Trends Pharmacol. Sci.*, **2006**, 27, 8, 402-409
(2) O. M. Downer, R. E. G. Marcus, N. R. Zürcher, and J. M. Hooker, *ACS Chem. Neurosci.*, **2020**, 11, 15, 2192-2200
(3) Y. Guo *et al.*, *Science*, **2015**, 347, 6221, 551-555
(4) F. Li, J. Liu, Y. Zheng, R. M. Garavito, and S. Ferguson-Miller, *Science*, **2015**, 347, 6221, 555-558
(5) M. Jaremko, Ł. Jaremko, G. Jaipuria, S. Becker, and M. Zweckstetter, *Biochem. Soc. Trans.*, **2015**, 43, 4, 566-571
(6) C. Lefebvre, J. Klein, H. Khartabil, J. -C. Boisson, and E. Hénon, *J. Comput. Chem.*, **2023**, 44, 20, 1750-1766
(7) L. Issop, L. Duma, S. Finet, O. Lequin, and J.-J. Lacapère, *Biochimie*, **2024**, 224, 16-28

O5 - In Silico Design and Prediction of Structural Properties of Dimerization Interfaces of Drosophila Melanogaster Gluthatione Transferases

Nicolas Petiot*[1], Mathieu Schwartz, Patrice Delarue, Patrick Senet, Jean-Marie Heydel, Fabrice Neiers, and Adrien Nicolaï
[1] Laboratoire Interdisciplinaire Carnot de Bourgogne – Université de Bourgogne EA7317, CNRS – France

Glutathione Transferase (GST) is a superfamily of ubiquitous enzymes, multigenic in several organisms. Typically, GSTs function as homodimers, where the dimerization interface plays a crucial role in maintaining structural stability and catalytic activity (1). The primary biological role of GSTs is to catalyze the conjugation of reduced glutathione (GSH), their cofactor, to hydrophobic xenobiotic centers. Each GST subunit contains two distinct binding sites: a highly conserved Glutathione-binding site (G-site) and a more variable ligand-binding site (H-site), which accommodates diverse substrates. In this study, we focus on the model organism *Drosophila melanogaster* (fruit fly, *D. mel*), which comprises 42 GST sequences grouped into six classes, collectively known as its GSTome. Through a comprehensive structural analysis of the *D. mel* GSTome (2), we identified key residues and motifs critical for the dimerization process and structural stability of GSTs. Additionally, based on the sequence conservation within the *D. mel* GSTome, we performed Monte Carlo Sampling in Sequence Space (MCSS) to optimize the dimerization interfaces of GST enzymes. Single-mutation structures were predicted using AlphaFold2-multimer. Optimized sequences and structures were evaluated and ranked according to energy minimization in vacuum.



From sequence distributions, we identified new dimerization motifs along with their corresponding structural designs, comparing them to known GST dimerization motifs such as Wafer and Clasp. Finally, we validated the stability and dimerization energies of the designs using classical all-atom Molecular Dynamics simulations in explicit solvent. We then constructed free energy landscapes using both coarse-grained and side-chain dihedral angle internal coordinates. This approach allowed us to correlate local conformations in the dimerization interfaces with interaction energies between subunits. As a next step, GST designs will be synthesized and experimentally validated through *in vitro* testing to confirm the impact of sequence modifications on stability. This methodology will also be extended to investigate protein-ligand interactions within GSTs.

(1) M. Schwartz, *et al.*, *Biomolecules*, **2024**, 14, 758
(2) N. Petiot, *et al.*, *Biomolecules*, **2024**, 14, 759

O6 - The lipid environment of membrane proteins modulates their function: the example of P2Y12 and SR-B1

Florentin Allemand*[1,3], Jennifer Lagoutte-Renosi[2], Siamak Davani[2], Christophe Ramseyer[3]
[1] Laboratoire de Biologie Structurale de la Cellule, Ecole Polytechnique, CNRS
[2] SINERGIES, Université Marie et Louis Pasteur, CHU Besançon
[3] Laboratoire Chrono-environnement (UMR 6249), CNRS, Université Marie et Louis Pasteur

A majority of drugs on the market target membrane proteins, especially G protein-coupled proteins, which are the target of more than a third of drugs [1]. These proteins are embedded in complex lipid membranes composed of a variety of lipids in terms of lipid heads and tails. These lipids organize themselves to form domains exhibiting different properties in these membranes. The proteins embedded in these membranes are sensitive to these properties. Furthermore, the properties of these membranes can be affected by the insertion of molecules known as membranotropic molecules. This is particularly the case for two antiplatelet agents, Ticagrelor and Prasugrel, which target the P2Y12 receptor of the G protein-coupled receptor type. These receptors are located in the platelet plasma membrane, more specifically in the arachidonic acid-enriched domain [2]. Models of these domains were simulated for 200 ns by molecular dynamics with 4 drug molecules – 2 per leaflet – inserted into them. This revealed that ticagrelor increases the lipid order of lipid from these domains, and to a lesser extent, prasugrel as well. Similar molecular dynamics simulations were performed with the target of these drugs, the P2Y12 receptor, embedded in these models. Combined with an ensemble docking approach, they revealed that the rigidification of the lipid environment modulated its binding with Ticagrelor and Prasugrel. In the case of Ticgarelor, this promotes its binding to P2Y12, as has been demonstrated in vitro [3], unlike Prasugrel. Another example illustrating the importance of the lipid environment on membrane proteins is the SR-BI receptor. This receptor is expressed by liver cells to bind high-density lipoproteins in order to unload them into cholesterol for elimination [4]. This receptor was simulated for 200 ns by molecular dynamics in two types of lipid environment: pure POPC, and lipid raft type. The lipid raft-like environment is far more favorable to this receptor and allows the receptor to anchor in the lipid bilayer as predicted by experimental data, which is not the case in the pure POPC model. These two examples demonstrate the importance of the lipid environment on membrane proteins. Moreover, the properties of these environments can be modified by small membranotropic molecules such as Ticagrelor and Prasugrel.

(1) K. Sriram, P. A. Insel, *Mol. Pharmacol.*, **2018**, 93(4), 251-258
(2) F. Allemand, S. Yesylevskyy, J. Lagoutte-Renosi, S. Davani, C. Ramseyer, *Biochim. Biophys. Acta - Biomembranes*, **2025**, 1867(1), 184402
(3) K. Pyrshev, F. Allemand, V. Rabani, S. Yesylevskyy, S. Davani, C. Ramseyer, J. Lagoutte-Renosi, *Br. J. Pharmacol.*, **2024**, 181(21), 4369-4380
(4) H. R. Powers, D. Sahoo, *Curr. Atheroscler. Rep.*, **2022**, 24(4), 277-288

O7 - A quantum dynamical study of the cis-trans isomerization in Rhodospin

Roberto Marquardt*[1], Etienne Gindensperger, Souvik Mandal[1], Maitreya Haldar[1]
[1]Laboratoire de Chimie Quantique de Strasbourg (LCQS), CNRS UMR 7177, Institut de Chimie de Strasbourg, Université de Strasbourg

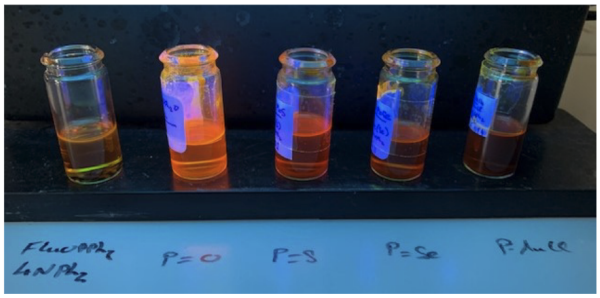
The photoisomerisation around a CC double bond is investigated quantum dynamically on the basis of a three mode two state model of the protonated Schiff base (PSB) in rhodopsin[(1,2)]. The original model is reviewed, the cis to trans isomerisation is studied in terms of time evolving wave packets and reaction probabilities and results are compared with the previous studies. Time dependent stimulated emisson and photoproduct absorption spectra are calculated. The generic results from the model are used to rationalize signatures of "vibrational coherence" evoked in experimental data[(3,4)].

Acknowledgement: Work supported by ANR, HPC-Strasbourg
Keywords: Rhodopsin isomerization, quantum dynamics, vibrational coherence
(1) E. Marsili, M. H. Farag, X. Yang, L. De Vico, M. Olivucci, *J. Phys.Chem. A*, **2019**, 123, 1710
(2) E. Marsili, M. Olivucci, D. Lauvergnat, F. Agostini, *J. Chem. Theory Comp.*, **2020** 16, 6032
(3) J. Léonard, I. Schapiro, J. Briand, S. Fusi, R. R. Paccani, M. Olivucci, S. Haacke, *Chem. Eur. J.* **2012**, 18, 15296
(4) M. Gueye, M. Paolino, E. Gindensperger, S. Haacke, M. Olivucci, J. Léonard, *Far. Disc.*, **2020**, 221, 299

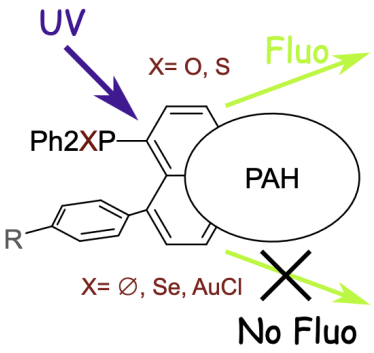
O8 - Rationalizing fluorescence properties of fluoranthenyl phosphines thanks to simple static theoretical approach

Guillaume Le Breton*[1], Julien Roger[1], Anne Pensel[2], Marie Cordier[2], Mureil Hissler[2], Jean-Cyrille Hierso[1], Pierre-Antoine Bouit[2], Paul Fleurat-Lessard[1]
[1]Institut de Chimie Moléculaire de l'Université de Bourgogne Europe
[2]Institut des Sciences Chimiques de Rennes

Being able to predict the fluorescence properties of molecules has been, remains, and will continue to be a central topic in theoretical chemistry. A wide range of techniques, with varying levels of complexity, can be employed to investigate the possible deactivation pathways that may suppress fluorescence — from the AI approach, which provides results without offering much explanation, to the time propagation of correlated vibronic states, which delivers detailed insights at the cost of significant computational and human resources. I will describe our efforts to rationalize the fluorescence properties of fluoranthenyl phosphine derivatives(1), in which oxidation of the phosphorus atom induces fluorescence. To this end, I employ relatively simple, inexpensive, well-established, and effective static approaches. This pedagogical presentation will show how we investigate two primary non-radiative deactivation pathways — Spin-Orbit Coupling (SOC) and Internal Conversion (IC)(2)— to estimate fluorescence potential using TDDFT calculations. Our approach has led to a deeper understanding of the system-dependent Photoinduced Electron Transfer (PET)(3) observed in these derivatives.



X= O, S, Se, AuCl



(1) C. Sire *et al.*, *Eur. J. Inorg. Chem.*, **2025**, 28(8), e202400721
(2) K. Veys *et al.*, *J. Chem. Theory Comput.*, **2023**,19(24), 9344-9357
(3) D. Escudero, *Acc. Chem. Res.*, **2016**, 49(9), 1816-1824

O9 - Creation of stable biomimetic nanopores in view of water sea desalination

Fatouma Hassan[1,2], Fabien Picaud[1]
[1] SINERGIES (Soins intégrés, Nanomédecine, IA & Ingénierie pour la Santé), Université Marie et Louis Pasteur, 16 route de Gray, 25000 Besançon, France
[2] Université de Djibouti, Croissement RN2-RN5, 1904 Djibouti, Djibouti

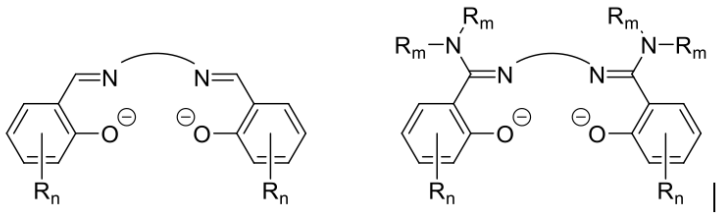
One of the major challenges of the 21st century is access to clean water. Its availability is expected to decrease in the coming years due to climate change, population growth, and pollution, leading us towards a potential shortage of potable water. Current water desalination technologies are limited due to their high costs and high energy consumption. Hence the urgent needs for sustainable solutions. Scientific research is beginning to explore ways of developing bio-inspired functional materials for water filtration and purification processes. In this work, we envisage the creation of artificial ion channels mimicking natural biological channels using high performance simulations. For this, we use a synthetic material (i.e. carbon nanotubes) to minimize energy consumption in a desalination system, coupled with a transmembrane polypeptide called gramicidin A (gA). Cautions have been taken to transfer proteins into artificial nanopores, as the environment differs from that of lipid membranes. We will present here the different phases of optimization of this novel biomimetic nanofluidic system, from the best carbon nanotube geometry to stabilize the polypeptide to the best conditions of voltage (from static to periodic) to discriminate ions through the channel and desalinate water at best.

Keywords : Biomimetic nanotechnologies, Carbon nanotubes, Gramicidin, Molecular dynamics simulation, Protein stability, Water diffusion

O10 - Theoretical investigation of FAlen-Zn complexes coordination: when causes are actually consequences

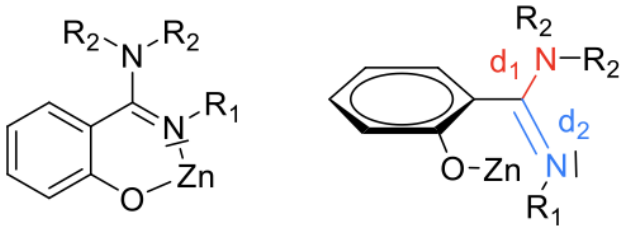
Jean-Thomas Pouzens*[1], Thu-Van Nguyen[1], Benjamin Théron[1], Lukas Vlk[1], Valentin Vaillant-Coindard[1], Cédric Balan[1], Jérôme Bayardon[1], Laurent Plasseraud[1], Yoann Rousselin[1], Paul Fleurat-Lessard[1], Raluca Malacea-Kabbara[1], and Pierre Le Gendre[1]
[1]Institut de Chimie Moléculaire de l'Université de Bourgogne Europe

Salen ligands are tetradentate N2O2 Schiff-bases. Their metal complexes used in several fields such as catalysis(1), chemical sensors(2) or energy storage(3). However, those complexes are sensible to hydrolysis, reduction of alkylation, reducing their efficiency. To overcome this, a new generation of ligand were designed with phenoxy-amidines replacing phenoxy-imines. This so-called FAlen ligand is more robust against reducing or nucleophilic agents and presents improved performances such as the (FAlen-κ^2)AlMe2 for ring opening metathesis (Scheme 1).(4)



Scheme 1: Salen and Falen ligands structures

FAlen ligands offer a great flexibility when it comes to the coordination. Indeed, they can express monodentate to tetradentate behaviours and become bridging to form dimers.(4) This flexibility comes with two main types of coordination: End-on and Side-on (Scheme 2). Moreover, this coordination might lead to an inversion of the bond length ($d_2 > d_1$) for specific FAlen-Zn complexes.



Scheme 2: End-on and side on coordination modes

We used DFT and Topological approaches FAlen-Zn complexes as well as different models based on phenoxy-amidine and phenoxy-imines to explain this unusual coordination mode. Our analysis reveals that amidines are not the main drivers of the side-on coordination. On the other hand, the bond length inversion depends on many parameters.

This work was supported by ANR (MORFAL, ANR-22-CE07-0011)
(1) S. Shaw, J. D. White, *Chem. Rev.*, **2019**, 119 (16), 9381-9426
(2) M. Strianese, D. Pappalardo, M. Mazzeo, M. Lamberti, C. Pellecchia, *Dalton Trans.*, **2020**, 49 (46), 16533-16550
(3) C. Freire, M. Nunes, C. Pereira, D. M. Fernandes, A. F. Peixoto, M. Rocha, *Coord. Chem. Rev.*, **2019**, 394, 104-134
(4) V. Vaillant-Coindard, F. Chotard, B. Théron, C. Balan, J. Bayardon, R. Malacea-Kabbara, E. Bodio, Y. Rousselin, P. Fleurat-Lessard, P. Le Gendre, *Inorg. Chem.*, **2023**, 62 (19), 7342-7352

O11 - Unveiling the Influence of Cavity-Shaped Diphosphanes on α-C4 Selectivity in Nickel(II)-Catalyzed Ethylene Oligomerization: A GFN2-xTB and IGM Approach

Sara Figueirêdo De Alcântara Morais*[1], Katrin Pelzer[2], Dominique Armspach[1], Yann Cornaton[1], Jean-Pierre Djukic[1]
[1] Institut de Chimie de Strasbourg – Université de Strasbourg, CNRS – 4 Rue Blaise Pascal, 67000, Strasbourg, France

Nickel(II) complexes with cis-chelating diphosphanes derived from cyclodextrins (CDs) have been demonstrated to act as active catalysts in ethylene oligomerization. The CD cavity is shown to influence both the catalytic activity and selectivity of the reaction, with but-1-ene being the major product.(1) To better understand the influence of the supramolecular environment on ethylene oligomerization, a theoretical study was conducted. Due to the size of the system (200 atoms), full DFT mechanistic studies are computationally challenging. Therefore, the semiempirical tight-binding method GFN2-xTB(2) was employed. A benchmark study comparing the GFN2-xTB approach to DFT (PBE-D3(BJ) functional) carried out on steps I to V (cf. Figure 1(a)) shows GFN2-xTB offers a good balance between computational efficiency and accuracy, suitable for the mechanistic study of this system. A mechanistic analysis following the scheme in Figure 1(a) was conducted for systems with and without the CD-cavity. Theoretical results show that the CD cavity enhances ethylene-Ni interactions consequently lowering the activation barriers and promotes α-C4 formation by restricting the mobility of the coordinated olefin. Independent Gradient Model(3) (IGM) analysis revealed the CD ligand increases non-covalent interactions with the substrate compared to the cavity-free ligand, enhancing the ethylene-Ni interaction through supramolecular confinement.(1)

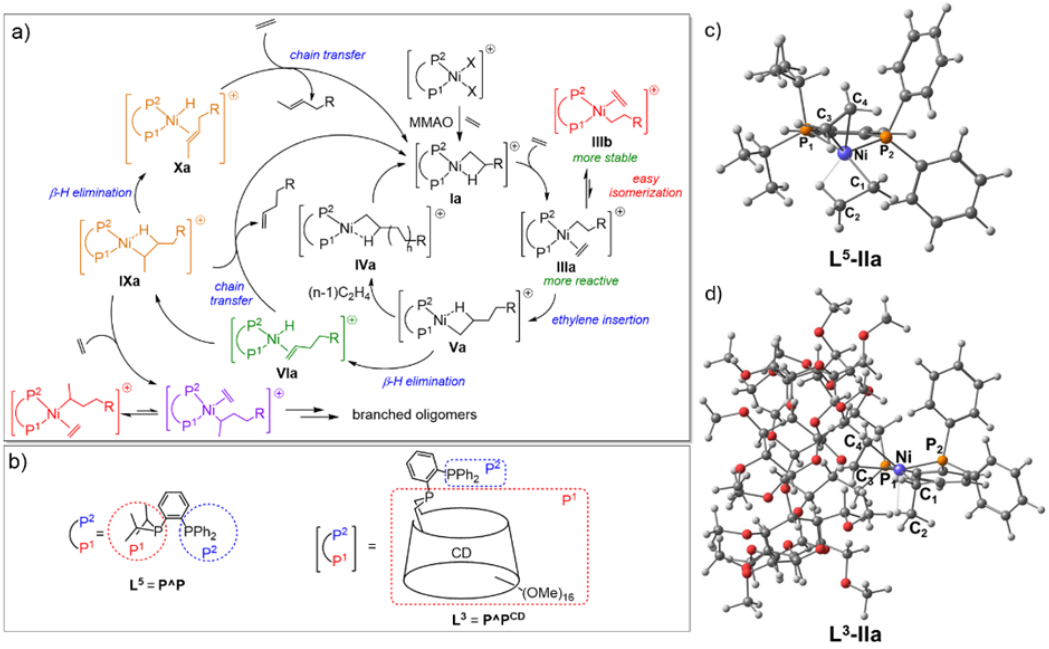


Figure 1: a) Scheme of Nill)-catalyzed ethylene oligomerization with the ethyl group coordinated in the active complex I trans to P1 (a, in black) or trans to P2 (b, in red). b) Scheme of the studied ligands without CD (left), and with CD (right). Optimized geometry of L-IIa (c) and L'-Ia (d) computed at the GF N2-xTB/ALPB(toluene) level of theory.

(1) Y. Li, S. F. de A. Morais, M. Han, T-A. Phan, G. Creste, M. Jouffroy, D. Matt, J-P. Djukic, Y. Cornaton, P. Braunstein, K. Pelzer, D. Armspach, *Chem. Eur. J.*, **2025**, e202501188
(2) S. Ehlert, M. Stahn, S. Spicher, S. Grimme, *J. Chem. Theory Comput.*, **2021**, 17, 4250-4261
(3) C. Lefebvre, J. Klein, H. Khartabil, J. C. Boisson, E. Hénon, *J. Comput. Chem.*, **2023**, 44, 1750-1766

O12 - Computational insight into the geometry of amidine-phenoxy early transition metal complexes

Mehmet Jahja*[1]
[1]ICMUB, Université de Bourgogne Europe, Dijon

The combination of phenoxy-imine (FI) ligands with Group 4 metal ions has proven to be one of the most efficient and versatile classes of olefin polymerization catalysts.1 Recently, our group developed a variant of the FI ligands by replacing the vulnerable imine function with an amidine group.2 These amidine-phenoxy (AF) ligands were then used to obtain (AF)2MX2 complexes (M = Ti, Zr) (Scheme 1, left). The solid-state structures of most of these complexes have been established by single crystal X-ray diffraction analysis. All the complexes showed a distorted octahedral geometry around the metal centre with the same O-trans, N-cis, X-cis configuration (isomer 1). Consistently, NMR spectroscopy of (AF)2MX2 complexes in solution shows that all complexes exist only as a symmetrical C2 isomer. This distinguishes AF ligands from their FI counterparts, which generally give Ti/Zr-FI complexes also as O-trans, N-cis, X-cis isomer in the solid state but as a mixture of isomers in solution. (FI)2MX2 and (AF)2MX2 complexes can theoretically exist in five isomeric forms (Scheme 1, right). For olefin polymerization, the ideal structure are isomers 1-3 which offer cis-positions for the growing polymeric chain and the incoming monomer. On the contrary, isomers 4 and 5 are inactive because they offer trans reactive positions which prevents the migratory-insertion step of the reaction. The nature of the isomer (1-3) has also a significant impact on the stereochemical outcome of the polymerization reaction when 1-substituted olefin is used (propene, styrene...). Therefore, it is important to have control over which isomer is formed..
These observations drove us to examine the stability and the interconversion of the isomers in FI and AF group 4 metal complexes with Density Functional Theory.
In this communication, we will show that seemingly contradictory experimental results come from the interplay between the electronic structure of the AF ligands and the steric hindrance of the R1 group.

Posters

P1 - 19F NMR study of the ligand-protein interactions - the case of the transmembrane protein TSPO

Luminita Duma*[1]
[1] Institut de Chimie Moléculaire de Reims - UMR 7312 – Université de Reims Champagne-Ardenne, Institut de Chimie - CNRS Chimie, Centre National de la Recherche Scientifique – France

Translocator protein (TSPO, 18 kDa), previously known as peripheral-type benzodiazepine receptor, is an evolutionarily conserved transmembrane protein involved in various physiological processes and patho-physiological conditions. The endogeneous TSPO ligand is a polypeptide of 9 kDa, but dipeptides with biological activity have been previously synthesized and characterized. Herein, we synthesized a phenyl alanine derived ligand with a 19F labelling which opens prospective for 19F-MRI and potential 18F-PET applications. We characterized the coexistence of two conformers and performed interaction studies with the recombinant mouse TSPO (mTSPO) in different membrane-mimicking environments using 19F NMR hence enabling structure/function characterizations. A change in the mTSPO environment from pure detergent to lipid/detergent mixture reveals different exchange rates between bound and free ligand forms. Competition experiments with the high-affinity drug ligand (R)-PK 11195 suggest that phenyl alanine derived ligand binds in the same protein cavity. To further enhance our comprehension of the impact of the membrane environment on ligand-protein interactions, we intend to compare the experimental findings with in-silico studies.

P2 - Beyond the usual suspects: On the importance of OH^-

Simon Chapuis*[1], Alain Chaumont[1], Rachel Schurhammer[1], Etienne Engler[1], Vahideh Alizadeh[2], Barbara Kirchner[2], Tom Frömbgen[2,3]
[1] Chimie de la matière complexe - Université de Strasbourg, Institut de Chimie - CNRS Chimie - France
[2] Mulliken Center for Theoretical Chemistry – Allemagne
[3] Max-Planck-Institut für Chemische Energiekonversion – Allemagne

To strengthen our knowledge on the reasons that lead to the formation of Deep Eutectic Solvents (DES) we have investigated the structure of three equimolar mixtures of Thymol with either Menthol, Borneol or Decanoic Acid via molecular dynamics (MD) simulations and quantum chemistry (QC) calculations. While the first two mixtures have been reported to form deep eutectic systems, the latter is known to only form an eutectic mixture. Each of these mixtures was simulated at least at 4 different temperatures in order to explore how its structural characteristics evolve with temperature. Spatial distribution functions reveal not only the presence of hydrogen bonds between the different components of each mixture but also the presence of OH^-.

P3 - Conception d'outils d'IA pour l'extraction automatisée d'informations et la prédiction des conditions optimales de réaction chimique

Ulrick Fineddie Randriharimanamizara*[1], Atif Anwer[1], Julien Roger[1], Fabrice Meriaudeau[1], Paul Fleurat-Lessard[1]
[1] Institut de Chimie Moléculaire, CNRS, Université Bourgogne Europe, Dijon

Les conditions de réaction chimique, telles que la température, le solvant et les catalyseurs, sont des paramètres critiques qui déterminent le succès et l'efficacité des transformations synthétiques, y compris le développement de médicaments ou de matériaux utiles. Cependant, l'identification des conditions optimales reste une tâche complexe, qui prend du temps et nécessite un effort expérimental important. Les récentes avancées dans les bases de données de réactions chimiques, combinées à l'essor des méthodes d'apprentissage automatique et d'intelligence artificielle, ont conduit à l'émergence d'outils informatiques visant à automatiser et à accélérer la prédiction des conditions de réaction. Malgré ces avancées, les modèles actuels souffrent souvent de performances limitées, en grande partie à cause de la mauvaise qualité et de l'incohérence des sources de données disponibles. Cette thèse vise à apporter de solution à ces problèmes par une double approche : (1) le développement d'un outil d'extraction d'informations automatisé pour extraire de manière fiable des informations de la littérature scientifique, et (2) la conception de nouvelles stratégies d'apprentissage automatique pour améliorer les méthodes existantes de prédiction de l'état de la réaction. Les résultats préliminaires mettent en évidence les principales limites des pipelines d'extraction de données et soulignent l'importance de la qualité des données pour la performance des modèles en aval. Ces connaissances guideront les prochaines étapes vers des cadres prédictifs plus robustes et généralisables.

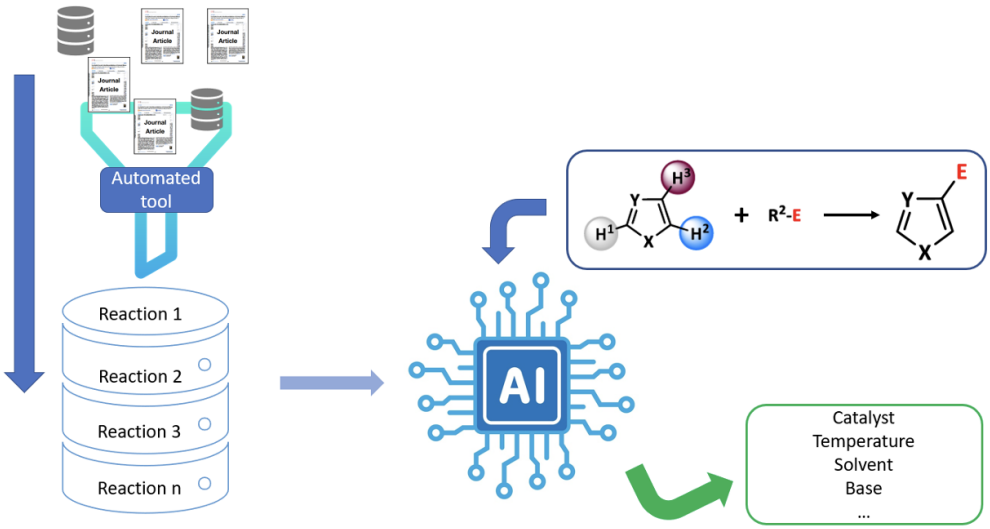


Figure 1: Project workflow.

Dans cette communication, je commencerai par énumérer les principaux inconvénients des méthodes actuelles utilisées pour extraire des molécules d'articles scientifiques et j'expliquerai comment nous avons résolu certains d'entre eux. Aussi, je présenterai les résultats préliminaires pour les modèles de prédictions de conditions réactionnelles.

(1) Z. Wang, K. Lin, J. Pei, L. Lai, *Chem. Sci.*, **2025**, 16, 854-866
(2) V. A. Afonina, *et al.*, *Int. J. Mol. Sci*, **2021**, 23, 248-248
(3) V. Voinarovska, M. Kabeshov, D. Dudenko, S. Genheden, I. V. Tetko, *J. Chem. Inf. Model.*, **2023**, 64, 42-56

P4 - DNA compaction regulation by the SIRT6 deacetylase: insights from molecular dynamics

Yuya Qiu[1], Gabor Papai[2], Adam Ben Shem[2], Emmanuelle Bignon*[1]
[1] Laboratoire de Physique et Chimie Théoriques – Institut de Chimie - CNRS Chimie, Université de Lorraine, CNRS – France
[2]Institut de Génétique et de Biologie Moléculaire et Cellulaire – Université de Strasbourg, Institut National de la Santé et de la Recherche Médicale : U964, CNRS, Université de Strasbourg : UMR7104, Institut National de la Santé et de la Recherche Médicale : U1258 – France

Sirtuins are a class of NAD-dependent histone deacetylases that regulate important biological pathways in prokaryotes and eukaryotes. This enzyme family comprises seven members, named SIRT1 to SIRT7. Among them, Sirtuin 6 (SIRT6) is a human sirtuin that deacetylates histone H3 and plays a key role in DNA repair, telomere maintenance, carbohydrate and lipid metabolism, and lifespan. SIRT6's structure consists of a zinc finger domain, a Rossmann fold domain containing the NAD+ binding site, and disordered N-terminal and C-terminal (CTD) extensions. The specific role of the CTD on SIRT6 interaction with nucleosomes for histone deacetylation remains unclear. Here, we resort to extended molecular dynamics simulations to uncover the dynamical behavior of the full-length SIRT6 bound to a nucleosome core particle. Our simulations reveal that the CTD preferentially interacts with DNA at the entry/exit point near the enzyme's docking site, exhibiting a variety of different binding modes. In specific cases, the CTD participates to the promotion of DNA unwrapping, also modulating the accessibility of target lysine residues located near the H3 histone core to SIRT6's active site. This work provides new structural insights into the binding process of the full-length SIRT6 to a nucleosome core particle, highlighting its participation in DNA unwrapping and lysine accessibility promotion.

P5 - Investigations of the Intermediate Scattering Function for a 1D Mathieu Potential

Mohammad Amini Valashani*[1], Roberto Marquardt[1]
[1] Laboratoire de Physique et Chimie Théoriques – Institut de Chimie - CNRS Chimie, Université de Lorraine, CNRS – France

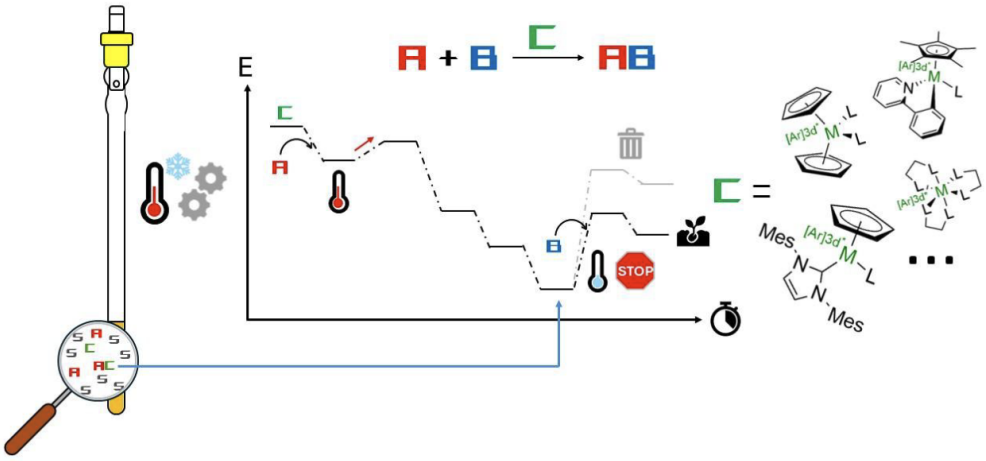
An interpretation of the Intermediate Scattering Function (ISF) as a quantum mechanical correlation function between two thermal wave packets has been recently proposed(1). This interpretation is relevant for the study of the diffusion of particles at the nanoscopic scale. It entails a method to calculate the ISF on a purely quantum dynamical basis using stochastic phases of the wave function. In this presentation an investigation is carried out with the aim to elucidate the effect of the stochastic averaging induced by the thermal wave packets.

(1) Bindech *et al.*, *arXiv*: 2407.03067, **2024**

P6 - Methodological approach to tackle mecanistic studies of homogeneous catalysis with 3d transition metal complexes : case study of hydroboration catalyzed by an Ni(+II) complex

Lucas Loir-Mongazon*[1], Yann Cornaton[1], Jean-Pierre Djukic[1]
[1] Institut de Chimie de Strasbourg, CNRS, Université de Strasbourg

Homogeneous catalysis involving chemical transformation of two reagents with a transition metal organometallic pre-catalyst in a one-pot synthesis process is an unmissable production strategy in the chemical industry of all kinds. Similarly, the most modern of these catalysts are developed with compelling earth-crest abundant 3d row metals as metallic center for economic motivation. Unveiling the mechanism of such chemical reaction would allow chemists to design more efficient pre-catalysts where understanding their behavior and fate should always be considered for environmental and profitable purposes. However, it can be quite puzzling to tackle this system as those three bodies can interact with each other in a gigantic number of potential processes and in tangled pathways. It should also not be neglected that the use of 3d transition metal complexes as catalysts implies treating them more cautiously due to their weak bonding character and predisposition to oxidation, often leading to parasitic reactions or decomposition. This latter aspect can hence make the trapping of any intermediates, keys to validate any mechanism, quite difficult and tedious. To illustrate this problematic, the activation mechanism of the hydroboration catalysis of styrene by catecholborane with a Nickel(+II) complex was investigated. To deal with this challenge, an approach of different experimental kinetic studies at inert atmosphere and various low temperatures followed by NMR was realized. DFT calculations were also performed and corroborated by isothermal titration calorimetry to model the thermodynamic and kinetic of the reaction. A metal-hydride complex was virtually trapped by cooling the reactive medium, stopping the evolution of the system, allowing long NMR analysis. This speculated intermediate is also supported by the DFT calculations and could correspond to one of the catalytic activated species of the reaction.



(1) L. Morán-González, A. L. Burnage, A. Nova, and D. Balcells, *ACS Catalysis.*, **2025**, 15 (11), 9089-9105
(2) Hsu, C.-W. CAS, 2023. https://www.cas.org/resources/cas-insights/understanding-power-catalysis (accessed 2025-06-11)
(3) J. V. Obligacion, P. J. Chirik, *Nature Rev. Chem.*, **2018**, 2, 15-34

P7 - Multiscale Modelling of DSB-Derivative Photothermal Transducers Forming Membranes Channels

Filippo Brunetti*[1], Mariachiara Pastore[1], Francois Dehez[1]
[1] Univesité de Lorraine, CNRS, Nancy

The controlled transport of ions and molecules across lipid bilayers via specific channels is a crucial mechanism for living cells. In the context of phototherapy, modulating the activity of membrane channels by light irradiation in a safe and controlled way is a promising route towards developing new therapeutic strategies beyond optogenetics. Dicyano-distyryl-benzene (DSB) derivatives serve as effective 2 photon-absorption photothermal transducers and have the unique ability to self-assemble within lipid membranes, potentially forming water or ion channels. The goal is to gain a better understanding of the self-assembly mechanisms and channel formation of DSB derivatives. For this purpose, a multiscale modelling approach is employed. Density Functional Theory (DFT) and Time-Dependent DFT (TDDFT) calculations are used to investigate the photophysical properties of both individual dyes and their aggregates, specifically the theoretical UV-vis absorption spectrum. Additionally, a transition density analysis was performed on the first two excited states. Molecular Dynamics (MD) simulations further explore the conformational space of DSB derivatives in solution and inside the lipid membranes, assessing the stability of the aggregates in solution and the effect of the environment on the conformation. The computational findings are then compared with experimental data to validate the methodologies used

P8 - Rethinking Chemical Bonding and Interaction Analysis with IGMPlot: A Comprehensive Platform to Understand, Teach, and Innovate

Hassan Khartabil*[1], Akilan Rajamani[1], Jean-Charles Boisson[2], Corentin Lefebvre[3], Julien Pilmé[4], Éric Hénon[1]
[1] Université de Reims Champagne-¬Ardenne, CNRS, ICMR, UMR 7312, Reims,
[2] Université de Reims Champagne-Ardenne, LICIIS / LRC CEA DIGIT, Reims, France
[3] Université de Picardie Jules Verne, LG2A, UR 7378, Amiens, France
[4] Sorbonne Université, LCT, UMR 7616, Paris, France

IGMPlot (available at http://igmplot.univ-reims.fr) is an open-source program designed to facilitate the study of molecular interactions across organic, inorganic, and biomolecular systems. It can fast-track the identification and visualization of both covalent bonding patterns and non-covalent interaction networks. IGMPlot provides a wide range of analysis tools: 2D interaction plots, 3D isosurfaces, quantitative indices such as δg, IBSI, PDA, DOI, as well as critical point descriptors. One of the key recent developments is the implementation of the ELF&IGM method, which combines the strengths of the Electron Localization Function and the Independent Gradient Model approaches. Accordingly, interaction regions are evaluated more rapidly and precisely, even in large and complex molecular assemblies. This makes it particularly valuable for systems such as protein-ligand complexes, metal-organic frameworks, or supramolecular assemblies. Overall, IGMPlot provides researchers with a powerful and efficient platform for characterizing interactions over a broad range: from non-covalent to covalent bonding and at low computational cost.

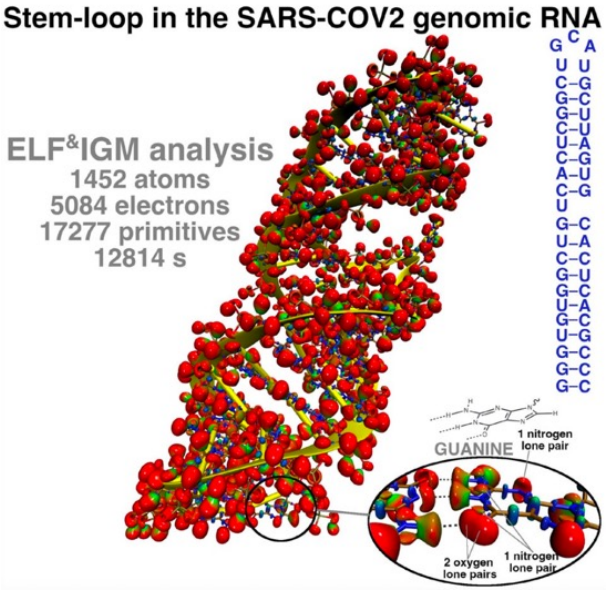


Figure 1: ELF&IGM RNA strand investigation ; 0.83 ELF isosurface colored with the IGM Γg(r) descriptor value using a BGR color scheme in the range [0.2:0.8]. Electron density derived from a wave function obtained from DFTB calculations

C. Lefebvre, J. Klein, H. Khartabil, J.-C. Boisson, E. Hénon, *J. Comp. Chem.*, **2023**, 44, 1750-1766
C. Lefebvre, G. Rubez, H. Khartabil, J.-C. Boisson, J. Contreras-García, E. Hénon, *Phys. Chem. Chem. Phys.*, **2017**,19, 17928-17936
C. Lefebvre, H. Khartabil, J.-C. Boisson, J. Contreras-García, J.-P. Piquemal, E. Hénon, *Chem Phys Chem*, **2018**, 19, 724-735
M. Ponce-Vargas, C. Lefebvre, J.-C. Boisson, E. Hénon, *J. Chem. Inf. Model.*, **2020**, 60, 268-278
J. Klein, H. Khartabil, J.-C. Boisson, J. Contreras-García, J.-P. Piquemal, E. Hénon, *J. Phys. Chem. A*, **2020**, 124, 1850-1860
C. Lefebvre, H. Khartabil, E. Hénon, *Phys. Chem. Chem. Phys.*, **2023**, 25, 11398-11409
H. Khartabil, A. Rajamani, C. Lefebvre, J. Pilmé, E. Hénon, *J. Comp. Chem.*, **2025**, 46: e70146

P9 - Theoretical Investigation of Bioinspired NNN-Pincer Iron Complexes for Photoelectrochemical C–H Bond Functionalization

Charles Willig*[1], Xavier Assfeld[1], Mariachiara Pastore[1]
[1] Laboratoire de Physique et Chimie Théoriques – Institut de Chimie - CNRS Chimie, Université de Lorraine – France

One of the holy grails of synthetic chemistry is the activation of CH bonds using cost-effective methods. Due to the high bond strength and chemical stability, CH bond activation usually requires harsh conditions, energy-intensive processes and the use of catalysts based on expensive (rare) transition metals. Our ultimate aim is to develop new catalysts based on earth abundant metal complexes, capable of activating CH bonds using solar energy. The photoelectrochemical approach is indeed both cost-efficient and operable under mild conditions. The NNN-Pincer Iron Complexes(1) that we are studying is bioinspired by metalloenzymes like cytochrome. When oxidized, the complex catalyzes the desired reaction. We will present in this lecture the preliminary steps of this study, focusing on two critical points. First, these Fe(III) complexes can exist in different spin states (high, intermediate and low spin arrangements), and it is essential to accurately describe, at DFT level, their geometries and relative energies. Second, since the photo(electro)chemical Fe(III)/Fe(IV) oxidation of the iron-pincer complex initiates the catalytic cycle, accurately predicting this redox potential considering solvent and ligand modifications is essential for guiding molecular design. To address these challenges, we performed benchmark calculations to identify the most reliable level of theory that balances accuracy and computational cost. Computed spin states and redox potentials will be presented and discussed.

(1) J. Han, L. Tan, Y. Wan, G. Li, S. N. Anderson, *Dalton Trans.*, **2022**, 51, 11620-24