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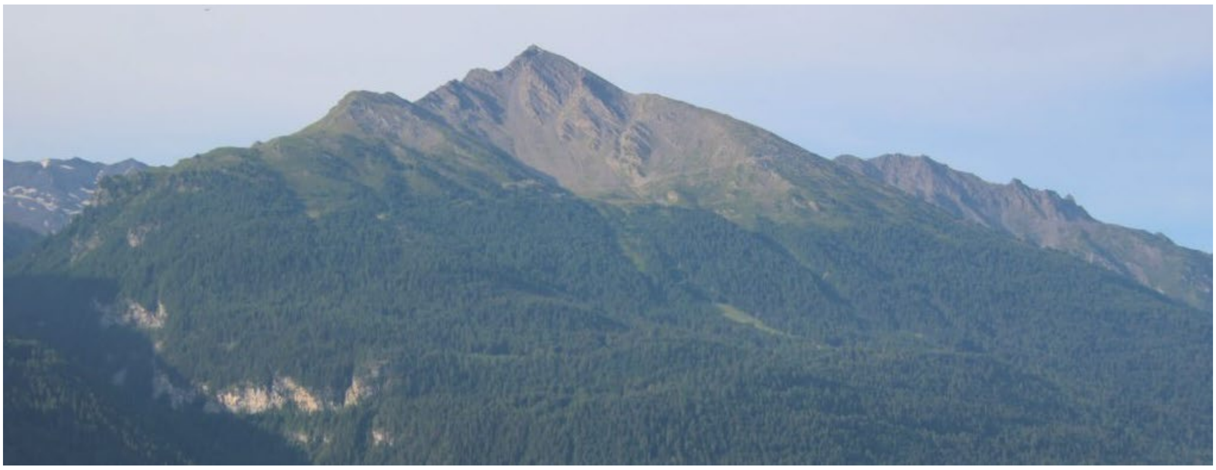
RCP2025 :

Rencontres de Chimie Physique 2025

15-17 sept. 2025 Aussois (France)



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PROGRAM

Monday, September 15th

14h00 - 15h30	Registrations
15h30- 15h45	Oppenong
15h45 - 16h15	Prix Chercheur confirmé : C. Georges *Does the interfacial chemistry of atmospheric aerosols lead to the production of hydroxyl radicals?*
16h15 - 16h30	O1 : Yao Qiwei *A Film of Hydrophobic Cations Reshapes the Electric Double Layer at the Metal/Water Interface*
16h30 - 16h45	O2 : Boukeke-Lesplulier Thomas *Exploring the mechanisms of damage of biomolecules upon ionising irradiation with numerical simulations*
16h45 - 17h00	Break and Posters
17h00 - 17h15	O3 : Triestram Léna *Simulating phase transitions in ZIF-4 using a machine learning potential*
17h15 - 17h30	O4 : Bowles Jessica *Raman spectra of silicic acids through classical polarisable molecular dynamics*
17h30 - 17h45	O5 : Habak Anna Maria *Synthesis of ferrocene derivatives as novel posolytes for energy storage*
17h45 - 18h00	O6 : Tetenoire Auguste *Multipodal Au–C grafting of calix[4]arene molecules on gold nanorods*
18h00 - 19h00	Posters
19H30	Dinner

Tuesday, September 16th

8h30 - 9h00	Prix de thèse : J. Vaz Ramos *Design of magnetic iron oxide/graphene based nanomaterials for the efficient and selective removal of polycyclic aromatic hydrocarbons from the environment*
9h00 - 9h15	O7 : Knapik Joachim *Simulation of a vibrational spectrum within a Quantum Computing framework*
9h15 - 9h30	O8 : Plazanet Marie *Structure and dynamics in Surfactant-free microemulsions*
9h30 - 9h45	O9 : Noman Syed *Electrochemical study of bio-polymer lignin: modification and valorization*
9h45 - 10h00	O10 : Dagnelie Romain V. H. *Diffusion of selenide in clay rock: an experimental journey at the crossroads between environmental sciences and radiochemistry*
10h00 - 10h15	O11 : Jiang zhiwen *Direct time-resolved study of the interfacial reaction mechanism of metal-based catalysts in the CO2 conversion*
10h00 - 10h30	Break + Poster
10h30 - 11h00	Invited Speaker : V. Vallet *Quantum-Chemical Insights into Actinide Bonding and Spectroscopy: 5f/6d Orbital Contributions, Spectral Signatures, and Volatility*
11h15 - 11h30	O12 : Courtiel Maïa *Modeling Water Clusters with Deep Neural Network Potentials*
11h30 - 11h45	O13 : Haq Marium *Molecular Investigation of the Interaction of Fluorescent Probes with Early Protein Aggregates*
11h45 - 12h00	O14 : Hoang Thi Hieu *Biomass conversion to added value products under Visible light excitation of Metal Halide Perovskites supported hollow spheres*
12h00 - 12h15	O15 : McDonald Peter *Elucidating the complex photophysics of luminescent donor-acceptor keto-coumarins*
12h15 - 12h30	O16 : Nushi Enida *Experimental study on the uptake of gaseous molecular iodine by atmospheric droplets*
12h30 - 14h00	Lunch

14h - 14h30	Prix Jeune Chercheur : V. Gonzalez *Deciphering the synthesis, formulation and alteration of historical pigments at the multi-scale*
14h30 - 14h45	O17 : Raju Maria Sara *Raman Optical Activity and ECD-Raman in Chiral Transition Metal Complexes*
14h45 - 15h00	O : 18Tsybizova Alexandra *Tautomerism and Conformational Effects in Protonated and Copper(I)-Coordinated Bis(oxazoline) Ligands: Insights from IRMPD Spectroscopy and DFT*
15h00 - 15h15	O19 : Boyer Emeline *Modeling the Vibrational Circular Dichroism spectroscopy of Phenylcyclohexanediol and Ionic Liquids to probe solvation properties*
15h15 - 15h30	O20 : Grill Justin *Advanced modelling of nonlinear optoelectronic properties of functionalized CdTe quantum dots using machine learning combined with DFT*
15h30 - 15h45	O21 : Sandre Olivier *Production and study of model nanoplastics by top-down and bottom-up methods for environmentally relevant studies*
15h45 - 16h15	Break + Posters
16h15 - 16h45	Invited Speaker : D. Rebiscoul *How the behavior of water and ions in confinement explains the evolution of nanoporous materials in solution*
16h45 - 17h00	O22 : Vangheluwe Raphaël *Accelerating the Structure Exploration of Diverse Bi–Pt Nanoclusters via Physics-Informed Machine Learning Potential and Particle Swarm Optimization*
17h00 - 17h15	O23 : Shaaban Tamara *Experimental Characterization and Theoretical Modelling of X-ray Absorption Spectra of Protactinium(V) Complexes*
17h15 - 17h30	O24 : Essylt Louarn *Electrochemical Analysis by mass spectrometry to study furfural reduction reactivity*
17h30 - 17h45	O25 : Gu Mingjun *Electrostatically Embedded QM/MM Study of the Potential-Dependent Reorientation of Pyridine on Au(111)*
17h45 - 19h00	Posters
19h30	Diner Gala

Wesnesday, September 17th

8h30 - 9h10	J. Perrin : M. Baaden *Taking Physical Chemistry into Cyberspace: From Computation to Immersive Discovery*
9h10 - 9h25	O26 : Desmedt Arnaud *ICONE: une nouvelle source compacte de neutrons pour la physico-chimie*
9h25 - 9h40	O27 : Herrero Cecilia *Fluids at an electrostatically active surface: Optimum in interfacial friction and hydroelectronic drag*
9h40 - 9h55	O28 : Ea Laura *Impact of the Host Polymer Viscoelastic properties on Magnetic Hyperthermia of Nanocomposites*
9h55 - 10h10	O29 : Merritt Isabella *Excited-state dynamics and thermal recovery of salicylidene-aniline photoswitches: a theoretical investigation*
10h10 - 10h30	Break + Posters
10h30 - 11h00	Prix de thèse : L. Godeffroy *Watching the electrochemistry of individual nickel-based nanoparticles by optical and X-ray microscopy*
11h15 - 11h30	O30 : Ben Amor Nada *Theory and Lattice Boltzmann Modeling of Complex Pollutants in Solution: Effect of the Porous Medium Heterogeneity on Adsorption and Transport*
11h15 - 11h30	O31 : Coste Amaury *Interplay of Structure and Dynamics in Solid Polymer Electrolytes: a Molecular Dynamics Study on poly(propylene carbonate)-based / lithium salt*
11h30 - 11h45	O32 : Abdelsater Mohammad *Microscopic view of hydrogen adsorption in size-variant nano-clays materials*
11h45 - 12h00	O33 : Senjean Bruno *Quantum algorithms for excited-state chemistry*
12h00 - 12h10	Awards
12h10	Lunch
14h00	Departure

INVITED LECTURES

Jean Perrin Conference
Taking Physical Chemistry into Cyberspace: From Computation to Immersive Discovery

Marc Baaden[1]

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Physical chemistry has always thrived at the intersection of ideas and instruments — spectroscopy, crystallography, and computer technology have each redefined what chemists can see and understand. However, as we enter the digital age, there is a danger that our field will fall behind in realising the full potential of cyberspace. Alongside today's familiar technologies such as 3D printing and data visualisation, new opportunities for immersive discovery are emerging, — where molecular modelling meets virtual reality, digital twins, and interactive exploration.

This talk will trace the historical interplay between technology and chemistry, highlighting both the leaps forward and the times when visionary ideas came too early and failed to catch on. Against this backdrop, I will discuss the breakthrough innovations of today: exascale computing, AI-driven predictions, integrative modelling and molecular digital twins that allow us to study systems from single proteins to complex membranes. These tools are changing the way we develop drugs, build synthetic channels, and imagine machines at the nanoscale.

The talk argues for a curiosity-driven adoption of new technologies, from visual analysis to interactive simulations and smart physical prototypes. By bringing physical chemistry fully into cyberspace, we open the door to new modes of discovery — where molecules can not only be calculated, but also experienced.

Prix Chercheur Confirmé 2024
Does the interfacial chemistry of atmospheric aerosols lead to the production of hydroxyl radicals?

Christian George[1]

[1]IRCELYON, Institut de recherches sur la catalyse et l'environnement
de Lyon, UMR5256, CNRS – UCBL, 2. av Albert Einstein
69626 VILLEURBANNE – France

Christian George a obtenu son doctorat à l'Université Louis Pasteur de Strasbourg et est directeur de recherche au CNRS. Il occupe actuellement la fonction de directeur adjoint de l'Institut de recherches sur la catalyse et l'environnement de Lyon (IRCELYON, CNRS – Université de Lyon). Son principal objectif scientifique est de comprendre les mécanismes des réactions hétérogènes se produisant dans les basses couches atmosphériques. En particulier, il étudie les réactions (photo)chimiques à l'interface air-aérosols, ainsi qu'à la surface des océans.

Christian George a été, ou est encore, membre de plusieurs comités scientifiques nationaux et internationaux, dont l'IGAC et l'iCACGP. Il est récipiendaire de deux projets « Advanced » de l'ERC (European Research Council) et est membre de l'Académie européenne des sciences.

Prix Jeune Chercheur 2024

Deciphering the synthesis, formulation and alteration of historical pigments at the multi-scale

Victor Gonzalez[1]

[1]PPSM, ENS Paris-Saclay, CNRS, 4 avenue des Sciences, 91190 Gif-sur-Yvette – France

Victor Gonzalez est chargé de recherche CNRS au laboratoire PPSM (ENS Paris-Saclay). Après avoir obtenu en 2016 son doctorat (Chimie, Sorbonne U.) mené au C2RMF, il a travaillé comme chercheur postdoctoral aux Pays-Bas, d'abord au sein du *Materials Science and Engineering Department* de TU Delft, puis du *Science Department* du Rijksmuseum, Amsterdam. En 2021, il a obtenu une bourse *Marie Sklowdoska-Curie* accueillie au PPSM, avant de rejoindre le CNRS en 2023.

Ses travaux portent sur la chimie des systèmes composites [pigment(s) inorganique(s) + liant(s) organique(s)] anciens, et plus particulièrement sur les mécanismes d’altération actifs au sein des formulations picturales historiques. Il mène ces études via la mise en œuvre de méthodes d’imagerie chimique à la multi-échelle, notamment fondées sur le rayonnement synchrotron.

Prix de thèse 2024

Design of magnetic iron oxide/graphene based nanomaterials for the efficient and selective removal of polycyclic aromatic hydrocarbons from the environment

Joana Vaz Ramos[1]

[1] *Institut de Chimie et Procédés pour l'Energie, l'Environnement et la Santé*
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25 rue Becquerel, 67087 Strasbourg – France

Docteure en physique et chimie-physique de l'Université de Strasbourg (décembre 2023), Joana Vaz Ramos a effectué sa thèse sous la direction de Sylvie Bégin à l'Institut de physique et chimie des matériaux de Strasbourg (IPCMS) et sous la co-direction de Stéphane Le Calvé à l'Institut de chimie et procédés pour l'énergie, l'environnement et la santé (ICPEES).

Sa thèse portait sur la conception des nanomatériaux composites recyclables constitués de graphène et de nanostructures magnétiques pour la captation des polluants et sur le développement des méthodes analytiques pour leur quantification et surveillance. Elle s'est intéressée à différents micropolluants organiques persistants, tels que les hydrocarbures aromatiques polycycliques (HAP), et aussi des polluants biologiques, comme les virus. Les nanomatériaux développés étaient très efficaces dans la captation des composés polyaromatiques dans l'eau et aussi prometteurs pour capter des virus. Son travail a conduit à cinq articles publiés, deux soumis et d'autres en cours de préparation. La qualité de son travail de thèse a été reconnue aussi par le comité de recherche de l'université de Strasbourg qui lui a décerné l'un des prix de thèse de l'année.

Prix de thèse 2024

Watching the electrochemistry of individual nickel-based nanoparticles by optical and X-ray microscopy

Louis Godeffroy[1,2]

[1]Université Paris Cité, ITODYS, CNRS, 75013 Paris - France
[2]Adresse actuelle : Nanoscale Solid-Liquid Interfaces, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 12489 Berlin - Allemagne

Louis Godeffroy est diplômé de l'ENS Paris-Saclay. Après une année de recherche pré-doctorale consacrée à l'étude de la réactivité électrochimique de nanoparticules individuelles par la méthode dite des « nano-impacts » dans l'équipe du Prof. Kristina Tschulik (Ruhr-Universität Bochum), il s'engage auprès du Dr. Frédéric Kanoufi (Université Paris Cité) pour préparer sa thèse de doctorat sur la même thématique.

Son projet de thèse consiste à coupler les microscopies électrochimiques (SECM, SECCM) à des techniques de microscopie optique super-résolues dans le but d'observer et de quantifier la réactivité de nanoparticules individuelles en temps réel, notamment dans le contexte de l'électrocatalyse et des batteries où la réactivité intrinsèque des particules actives est souvent difficile à dissocier de celle de l'électrode. Il est également à l'origine du développement d'algorithmes de traitement d'images innovants permettant d'exploiter tout le potentiel des vastes ensembles de données générés par les couplages multi-microscopiques.

Après avoir soutenu sa thèse le 6 octobre 2023, il rejoint l'équipe du Dr. Tristan Petit au Helmholtz-Zentrum Berlin où il développe actuellement la microscopie aux rayons X (STXM) en milieu liquide, notamment dans le but d'étudier les mécanismes de stockage de charge dans les MXenes.

Invited speaker

Quantum-Chemical Insights into Actinide Bonding and Spectroscopy: 5f/6d Orbital Contributions, Spectral Signatures, and Volatility

Valérie Vallet, Florent Réal, André Gomes[1]

Laboratoire, Université de Lille, CNRS, campus Cité Scientifique,
59655 Villeneuve d’Ascq - France

Understanding the chemistry and spectroscopy of actinides remains a major challenge due to the scarcity of experimental data, strong relativistic effects, and the complex electronic structure of 5f elements.

In this talk, I will present recent advances in quantum-chemical modelling of actinide systems, focusing on plutonium oxides, protactinium clusters, and uranium species in solution. Multi-reference relativistic methods allow us to reliably describe the thermodynamics and spectral signatures of volatile Pu compounds, shedding light on nuclear accident scenarios and contributing to the refinement of safety databases. Theoretical insights into the peculiar bonding of Pa(V) clusters highlight the role of 5f orbitals in stabilising structures absent in lighter homologues. Finally, vibronically resolved simulations of uranyl luminescence and U(IV) UV-vis spectra demonstrate how theory can complement experiments in unravelling actinide speciation in complex environments.

Overall, these studies illustrate the predictive power of quantum chemistry for actinide science, bridging microscopic bonding descriptions with macroscopic observables relevant to nuclear safety and environmental applications.

Invited speaker

How the behavior of water and ions in confinement explains the evolution of nanoporous materials in solution

Diane Rébiscoul[a], Hassan Khoder[a], Samuel Tardif[b], Markus Baum[a], Zijie Lu[b], Francois Rieutord[b], Vincent Larrey[c], Jacques Ollivier[d], Jean-Marc Zanotti[d], Fanni Juranyi[e], Kunyu Wang[a], Bertrand Siboulet[a]

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The understanding of the evolution of industrial or natural nanoporous materials filled of or in aqueous solution such as membranes, cementitious materials, polymers for fuel cells, biominerals, clay materials, secondary minerals, corrosion products and spent nuclear fuels, is important to explain and to predict their macroscopic behaviour. This macroscopic behaviour is governed by the spatial distribution, the transport and the chemical reactivity of water molecules and ions present in confined solution. More specifically, in single digit nanoconfinement (SDN), the system length scale crosses the classical key length scales describing energetics and equilibrium of electrolyte solutions next to surfaces. In this case, classical concepts fail to account for scale specific phenomena. Thus, to better understand the evolution of nanoporous materials, the descriptions of water molecules and ion properties need to be updated.

Here, we propose to illustrate how the understanding of water molecule and ion behaviors in SDN, can help to explain the evolution of nanoporous materials in solution. Our scientific approach is based on the determination of ion distribution and on the study of water dynamics in silica SDN filled of aqueous solutions with cations having various size and valence (XCl_n with n=1, 2 and 3). To reach this goal, we used a test vehicle that consists in 2, 3 and 5 nm-height silica nanochannels associated with an original characterization technique based on the interface hard X-ray reflectivity analysis. Here, we directly probed the transport of XCl_n solutions containing cations and their distributions in the nanochannels. Depending on the electrolyte, we observed nanochannels clogging and correlated this phenomenon to the specific ion effect. Coupled to the theoretical modeling of SiO-X and X-Cl interactions, we demonstrated that the interface, i.e. the surface cation excess density, is driven by the ionic interactions existing in nanochannels that depends on the charge, the size of the cation and its ability to form ion pairs. This result also explains the water dynamics at a picosecond timescale characterized by Quasi-Elastic Neutron Scattering in presence of the same electrolytes and confined in silica nanocylinders having a pore diameter of 2.6 nm. Indeed, while the monovalent cations exhibit weaker interactions with silica surface the strong interaction of divalent cations with silica surface significantly impacts the water dynamics in addition to the confinement and electrolyte effects. This pinpoints the importance of ion behavior within the interfacial layer and its impact on water transport in nanoconfinement.

To end, these results are significant for explaining various industrial or natural processes, particularly membrane filtration or glass alteration. As example, glass alteration rates measured on some borosilicate glasses in electrolyte solutions XCl_n (X = K, Cs, Ca) and driven by the reactive diffusion of water through the glass alteration layer, follows this order: $Ca \ll Cs < H_2O < K$. Here, the strong interaction of the divalent cation Ca^{2+} with the silica surface can also explain the strong decrease of the glass alteration rate in $CaCl_2$ solution compared to that in KCl and CsCl solutions.

ORALS

O1

A Film of Hydrophobic Cations Reshapes the Electric Double Layer at the Metal/Water Interface

Qiwei Yao[1]

[1]*Chimie Physique et Chimie du Vivant – Département de Chimie - ENS-PSL, Institut National de la Santé et de la Recherche Médicale, Sorbonne Universite, CNRS – France*

Recent studies have observed that the bulky hydrophobic cations are able to promote the rate of the hydrogen evolution reaction, such as the tetrabutylammonium (TBA+). The addition of bulky hydrophobic cations provides a new perspective for optimizing electrochemical reaction which requires a molecular-level understanding on the underlying changes in the interfacial environment. We have developed a THz ATR spectroelectrochemical cell to probe molecular-level details at the gold/water interface. This innovative setup reveals the potential-dependent formation of TBA-rich film at the Au/aqueous interface. Complementary molecular simulations demonstrate that above 0.6V versus Ag/AgCl, partial TBA+ desorption induced a coadsorption of TBA+/Cl- and interfacial rehydration. Our combined experimental-theoretical approach unravel the bulky hydrophobic TBA+ cations restructure the hydrogen bond network at the metal/water interface. This allows rationalizing at the molecular level the ions-induced structural changes at the interface that tune the catalytic performances.

O2

Exploring the mechanisms of damage of biomolecules upon ionising irradiation with numerical simulations

Thomas Boukéké-Lesplulier[a,b], Fabien Cailliez[a], Natacha Gillet[b], Aurélien de la Lande[a]

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[b] *Laboratoire de Chimie, Ecole Normale Supérieure de Lyon – Université de Lyon, CNRS UMR 5182, 44 allée d'Italie F69342 Lyon*

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Biomolecules are highly radiosensitive, yet the mechanisms of the radiative damage they undergo remain poorly known. In the context of the latest innovations in the field of radiotherapy (FLASH), we developed a protocol to study the ionising irradiation of biomolecules with fast ions. On the basis of experimental data [1], we probe it on the simulation of the collision of collagen mimetic peptides (CMP) in the gas phase with a C^{4+} cation at the Bragg peak energy (~ 1 MeV/a.u.). After a preliminary work on the protonation of CMP, we describe the electronic dynamics of the collision with real-time time-dependent auxiliary density functional theory (RT- TD-ADFT) [2]. We developed a tool to generate a pool of ion beam trajectories that extensively samples the irradiation (Figure 1). A complex absorbing potential models the ionisation through the emission of secondary electrons [3]. Thereby, we compute the energy deposited by the colliding ion and what remains of it in the vibrational modes of the molecule after ionisation and electronic relaxation. The subsequent damage is to be studied thereafter with non adiabatic dynamics simulations (QM/MM Ehrenfest). The same simulation protocol will be applied for the ionising irradiation of the nucleosome (DNAprotein complex), following the original interest for the biosystem that is the most relevant to radiotherapy. In either system, the limitation of the computational capacity calls for another approach. Therefore we work on machine learning code that may allow us to alleviate most of the RT-TD-ADFT calculations to compute energy depositions and electronic stopping powers (STOPPIA project, PNRIA). Finally, the damaged structures are studied with classical molecular dynamics. Regarding the nucleosome, we have already started to work with available structures bearing well-known radiative damage [4]. We focus in particular on DNA-protein cross-link between lysine residues located on histone proteins tails and guanine radical cation. The latter is a common product of radio-induced oxidation of DNA.

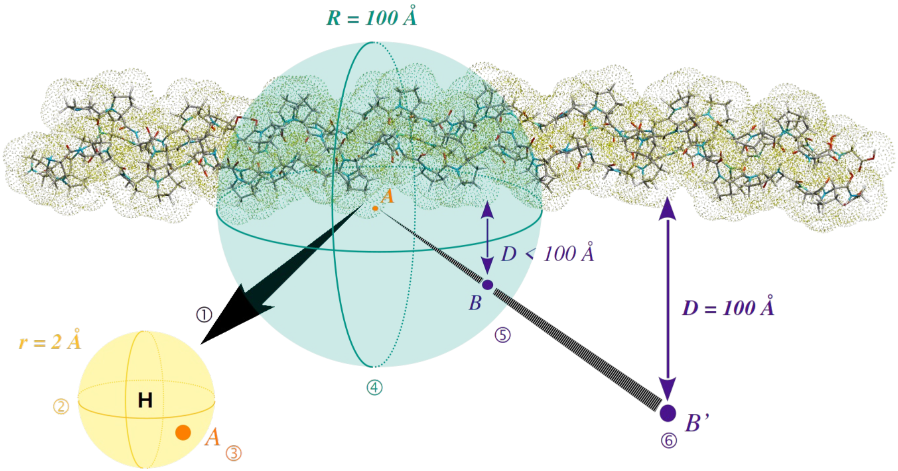

Figure 1: Sampling strategy to generate irradiation trajectories

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Simulating phase transitions in ZIF-4 using a machine learning potential

Léna Triestram[1] and François-Xavier Coudert[1]

[1] *Ecole Nationale Supérieure de Chimie de Paris - Chimie ParisTech-PSL – Université Paris sciences et lettres – France*

Zeolitic Imidazolate Frameworks (ZIFs) are a family of metal–organic frameworks composed of metal clusters bridged by imidazolate linkers. In this work, we are interested in simulating ZIFs based on Zn^{2+} ions. There exist several known topologies of this class of materials, most of them crystalline, but it is also known to feature amorphous structures which retain a high porosity. Many of these polymorphs have been characterised both experimentally (1) and in silico (2). Working on transitions between these phases allows us to explore the mechanisms of rearrangement of the structure during these processes.

We use a Machine Learning Potential (MLP) we generated, based on the MACE architecture (3) to simulate several phases of this material as well as phase transitions. We first present the simulation protocols: a melt-quench simulation which generates atomistic glass models from the ZIF-4 crystal and a simulation of the transition between two known phases: ZIF-4 and ZIF-4-cp-II.

The simulated structures need to be rigorously characterised; we thus used and developed methods to identify these phases. We present a neural-network classifier based on the local SOAP descriptor (4). Another way to classify phases is by using rings which are defined as closed loops with alternating imidazolate/cation. With these rings, we are able to see the change in topology (i.e., bond breaking or formation) as well as the change in the rings' shapes for transitions which do not involve topological changes. These tools are used as a means to pinpoint phase transitions in simulations.

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Raman spectra of silicic acids through classical polarisable molecular dynamics

Jessica Bowles[1], Fileto Rodriguez[1], and Frederik Tielens[1]

[1] *Vrije Universiteit Brussel [Bruxelles] – Belgique*

Raman spectroscopy uses a technique where the incident light is scattered by the sample. Most of the scattered light is at the same wavelength as the incident light source; this is called Rayleigh scattering. However a small amount of light is scattered at different wavelengths, and depends on the chemical structure of the system; this is called Raman scattering (1). As most vibrational spectroscopies such as infrared (IR) absorption, Raman can be used to study the structure through the vibrations of the molecule, furthermore, Raman can display IR inactive modes.

To support the interpretation of experimental measurements, theoretical predictions of Raman spectra are crucial. As an alternative to computational methods based on explicit descriptions of electronic structure such as DFT and ab initio molecular dynamics (2) and to circumvent their limited sampling capabilities in time and space, we have attempted to simulate the Raman spectrum directly from molecular dynamics trajectories employing a polarisable force field called AMOEBA (3). This force field offers a refined description of electrostatic interactions by accounting for both permanent atomic multipoles and induced atomic dipoles, the latter being essential for simulating Raman spectroscopy. The work here extends earlier efforts dedicated to the Raman spectrum of a single molecule (4) obtained through the Fourier transform of the autocorrelation of the polarisability tensor.

In this presentation, we expand the implementation of Raman spectroscopy using the AMOEBA polarisable force field in the Tinker software package (5) to silicic acids. Silicium is the second most abundant element, after oxygen, and is widely used in many fields. To study silicic acids, new parameters have been added to the AMOEBA force field specifically to describe them.

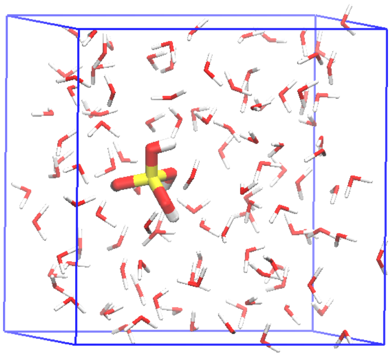

Figure : Periodic box of $Si(OH)_4$ in water

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O5

Synthesis of ferrocene derivatives as novel posolytes for energy storage

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During the past few decades, energy storage systems have attracted the attention of the scientific community due to the increased global need for sustainable energy which are, by nature, intermittent. While lithium-based batteries are widely used, they remain expensive, flammable, with a decrease of performances over time and with a limited lifetime. In the last years, aqueous redox flow batteries (AORFB) appeared as an appealing alternative due to their many advantages such as safety (non-flammable, non-explosive), low cost, sustainability and ability to decouple power and energy. [1] In this type of battery, electroactive species are one of the main components, used as electrolytes, dissolved in aqueous solution and stored in external tanks.

Despite years of study, there are currently only a few posolytes available for AORFB. Among them, ferrocene derivatives are particularly interesting because of their tunable reversible redox behavior, their stability and the non-critical nature of the iron present in their structure. However, their application in AORFB is limited by their low redox potential and limited solubility in water. To overcome these limitations, ferrocenes substituted with various solubilizing groups have been prepared. However, even though good solubilities have been achieved, decomposition (degradation with ligand dissociation, particularly when substituted by electron-withdrawing groups) remain a major problem. While the introduction of alkyl chain substituted by ammonium groups improves the stability of the compounds, it has also the consequence of lowering their redox potential. [2] Here, we report a new type of derivatives incorporating a judiciously chosen functional group (FG) between ferrocene and the solubilizing group (SG) for enhanced stability, along with a first evaluation as a posolyte in AORFB (*Figure 1*). The introduction of this functional group enabled the redox potential to remain relatively stable, regardless of the side chain bearing the solubilizing group. It also facilitates the introduction of additional substituents on the ferrocene core to improve its solubility in aqueous medium. In addition to monosubstituted compounds, 1,1'-disubsituted ferrocenes have been also investigated.

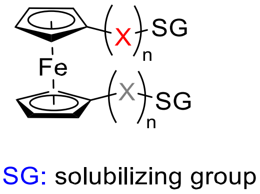

Figure 1: new ferrocene derivatives

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O6

Multipodal Au–C grafting of calix[4]arene molecules on gold nanorods

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The interface robustness and spatial arrangement of functional molecules on metallic nanomaterials play a key role in the potential applications of functional nano-objects. The design of mechanically stable and electronically coupled attachments with the underlying metal is essential to bring specific desirable properties to the resulting hybrid materials. In this context, rigid multipodal platforms constitute a unique opportunity for the controllable grafting of functionality [1]. The characterization of the interface in these hybrid materials is a challenge where modelization greatly helps the comprehension of experimental works. However, the limitations of the cluster size models computed with Density Functional Theory (DFT) method to reduce the computational effort are detrimental to the modelling of spectroscopic signatures.

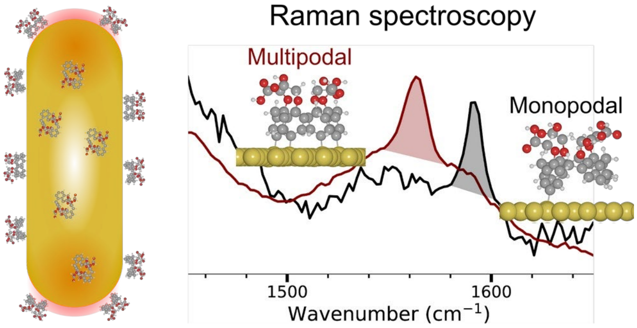

Figure 1: Left, scheme of calix[4]arene grafting on the surface of gold nanorod, probed by 785nm laser. Right, simulated Raman spectra for mono- and tetrapodal calix[4]arene grafted on gold surface.

In this work, we use Density Functional Tight Binding (DFTB) method to circumvent the limitation in size of the system and facilitate the comparison with experimental data. We observe that the multipodal grafting of calix[4]arene molecules on gold surfaces is very stable, with binding energies of several eV. Subsequently, we compute the Raman spectra of such a large system accounting for different gold surface indices. The simulated spectra allow the identification of the frequency of the normal modes associated with the grafting, and to distinguish between mono- and multipodal grafting, enhancing comprehension of the experimental spectra. The combination of experimental and theoretical results [2] provides, for the first time, an in-depth description of the interface between gold nanorods and a chemically grafted multipodal platform, establishing the foundations for the future design of robust and versatile platforms, later used as catalytic objects.

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Simulation of a vibrational spectrum within a Quantum Computing framework

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Quantum Computing is a promising solution to address many-problems more efficiently than Classical Computing, such as simulating vibrations in molecules quantum-mechanically. In contrast to electronic structure, the simulation of the vibrational structure of molecules with quantum bit (qubit)-based quantum computers is still in its infancy (1,2). The vibrational problems can be expressed with bosonic operators and they then, have to be encoded for the quantum computing simulation. Encodings of bosonic operators have only been explored recently. One cannot, directly encode the bosonic levels to the two states of a qubit. Hence, mapping a bosonic system on qubits is not straightforward, although some encodings have been developed to overcome this difficulty (3). We illustrate those encoding on a model system characterized by a one-dimensional double-well potential. The model is chosen to describe a large-amplitude motion exhibiting fine splitting of its eigenvalues due to deep tunneling (4). As one tries to simulate this model with quantum computing, unusual problems related to the expression of the bosonic operators can arise and deserve a special consideration. The impact of this problem and how to circumvent it, is presented along with a description of the Quantum Computing simulation of the model. Also, the efficiency of the quantum algorithm is inspected with respect to two representations of this model (5).

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Structure and dynamics in Surfactant-free microemulsions

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Ternary mixtures of oil, water and an hydrotrope can lead to complex and usable organization in terms of reactivity or solubility. This is the case of aqueous solutions of ethanol and oil, typically found in all kind of liquors, cosmetics or solvents for liquid-liquid extraction. The archetypical case of this family is the ternary mixture of water, ethanol and octanol. A rapid dilution of the monoalcohols binary mixture with water takes the system into the biphasic region, where a metastable emulsion of oil droplets forms, known as the " Ouzo " effect. Before reaching this phase, a thermodynamically stable region was also identified close to the critical point and described as pre-Ouzo region (1).
Our work aims at providing a quantitative description of the whole phase diagram of this system from a microscopic point of view. For this purpose, we mainly combined X-ray small angle scattering, quasi-elastic neutron scattering and PFG-NMR. Our investigations enabled us to characterize the organization and the diffusion of each molecular species in the various regions. The main structural parameters describing the different phases could be identified and related with the regimes observed in self and collective diffusion (2).
The fine tuning of such phases was eventually addressed in exploring temperature effects or subtle chemical substitution on the monoalcohol (3).

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O9

Electrochemical study of bio-polymer lignin: modification and valorization

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The continuous exploration of fossils to meet the global carbon demand has aggravated the already exacerbated environmental and climatic crisis and increasing political strife elicit the hunt for alternate renewable source of carbon. Lignocellulosic biomass has the potential to serve the purpose of replacing fossil feedstock for the acquisition of renewable carbon. Lignin is the second most abundant biopolymer on earth and is composed of phenylpropanoid units connected together via different linkages mainly including β-β, β-5, 4-O-5 and the weakest one β-O-4[1]. Breaking these bonds to depolymerize the lignin may pave pathway to the acquisition of value added platform chemicals to achieve carbon neutrality. However, this task is really challenging owing to the recalcitrant nature of lignin itself. Moreover, the isolation of lignin is an exhaustive process requires harsh conditions such as, acidic hydrolysis at elevated temperatures inflicts some conformational changes in the structure of lignin and producing condensed lignin which is quite stable and recalcitrant to depolymerization[2,3]. Nevertheless, by developing chemical modification protocols during isolation, these condensed lignin scenarios can be avoided[4,5] and contrast to the energy intensive conventional chemical methods, the lignin obtained can be depolymerized using electrochemical methods.

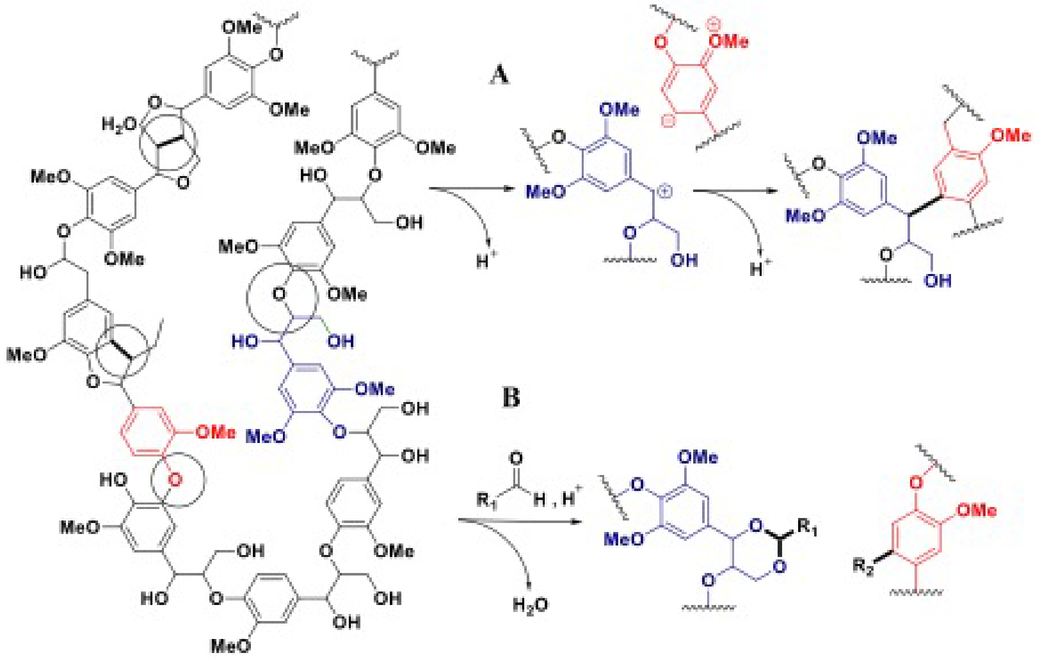

Figure: Schematic presentation of isolation of lignin; (A) in acidic conditions and (B) the same under the protection of aldehyde to avoid lignin condensation.

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O10

Diffusion of selenide in clay rock: an experimental journey at the crossroads between environmental sciences and radiochemistry.

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The knowledge of metal and radionuclide's migration is of interest in many industrial fields, such as environmental monitoring, or radioactive waste management. In this context, the migration of contaminant is measured in the barriers of interest such as soils or sedimentary rocks. Recent studies focus on anionic species which are especially mobile in reductive media (e.g. 36Cl$^-$, 129I$^-$, 79Se^{2-}) [1]. Among them, the case of selenium displays a rather complex chemistry, analogous to that of sulphur. The main species of selenium expected in CallovoOxfordian (Cox) clay rock should be HSe$^-$, and Se(0) solid phase (Cox, E_h ~ -0.2 V). However, data on these forms are still scarce due to their very low solubility and chemical stability in presence of Fe(II). This study focuses on the stability, retention and mobility of reduced forms of selenium expected in Cox clay-rock [2,3].

The specific chemistry of selenide species required the development of unusual techniques. In this presentation we will detail three experimental steps of this study. Firstly, the synthesis of 75Se radiotracer under reduced form was necessary, allowing measurements at the very low concentrations required (<< 10^{-10} M). Secondly, a handmade analytical procedure coupled blind chromatographic separation and gamma counting. This setup not only allowed the quantification of 75Se, but also provided insights on slow oxidative polymerization process (Fig. 1, left). Finally, retention and diffusion experiments were performed on the natural reducing media, i.e. in Cox clay rock. After 100 days of diffusion under anoxic glovebox, the diffusive profiles of Se were quantified in the rock, over six orders of magnitude [3]. This data evidenced the slow diffusion of a reduced form of selenium, slightly stabilized by the presence of hydrazine. The evolution of the selenium speciation indicated an oxidation process in the clay rock sample, eventually delayed by intermediate polymerization into polyselenide $(Se)_n^{2-}$, before precipitation into Se(0). Such case study was a challenging experimental journey at crossroads between radio-, analytical-, and physical-chemistry.

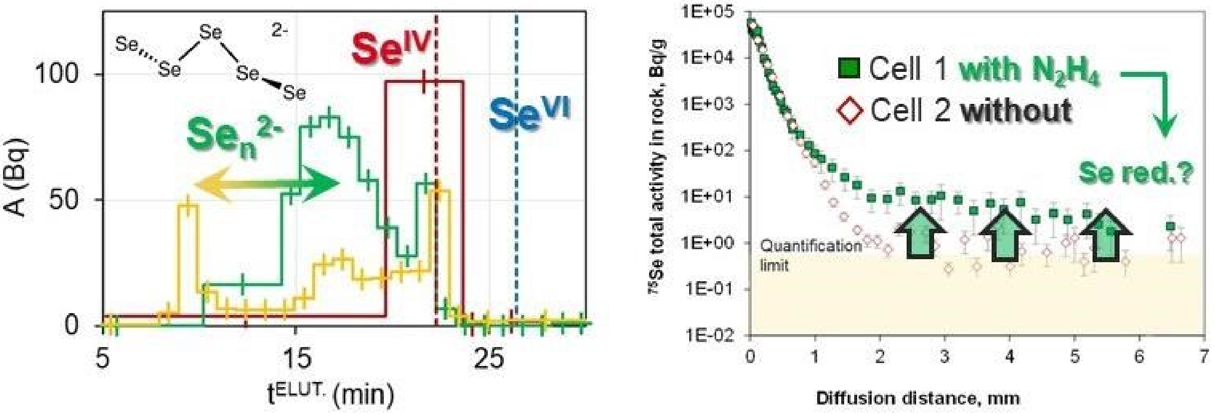

Figure : (Left) Elution chromatography of reduced source of 75-Se measured by gamma counting. (Right) Diffusion profile of 75-Se in a rock sample after100 days of diffusion. (Reprocessed from [3])

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Direct time-resolved study of the interfacial reaction mechanism of metalbased catalysts in the CO2 conversion

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Metal-based catalysts have attracted much attention due to their unique activity and selectivity in catalytic CO_2 reduction reactions. However, the transient identification of interfacial intermediates and the complex dynamic evolution of catalyst surfaces pose great challenges to revealing their reaction mechanisms.

In this study, we directly observed the transient intermediates and their initial electron transfer during catalytic CO_2 reduction processes on the surfaces of typical metal-based catalysts (Au, Cu, Ni) using picosecond pulse radiolysis. The interfacial elementary reactions and their kinetic behaviors are resolved. The developed multi-step pulse method also enables time-resolved monitoring of the dynamic evolution of the oxidation state of oxide-derived copper catalysts, systematically revealing the interfacial reaction mechanism of copper oxides in the catalytic CO_2 reduction reaction.

O12

Modeling Water Clusters with Deep Neural Network Potentials

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Understanding the structural and dynamical behavior of water clusters is still a central question as the mechanisms and physico-chemical phenomena occurring in such clusters can help us in gaining insight into the properties of liquid and solid water [1,2]. In 2017, K. Korchagina *et al.* [3] conducted a theoretical study on the $(H_2O)_{20\text{-}23}H^+$ clusters, successfully reproducing the shape of the experimental caloric curves and their size dependence. The simulations provided deeper insight into the nature of the phase transition, linking it to structural changes, water molecule dynamics, and proton mobility.

To extend this understanding to larger clusters and to achieve higher accuracy in the description of their structural and dynamical properties, more advanced simulation methods are required. However, the high computational cost of such approaches imposes severe limitations on the size and timescale that can be realistically explored.

In this work, we present a novel approach based on deep neural network potentials (DNNPs) build using the DeepMD-kit [4], to investigate large water clusters ($(H_2O)_{20\text{–}100}$) with density functional theory (DFT) accuracy, while incorporating nuclear quantum effects (NQE). We detail an iterative data generation based on an active learning procedure, starting at the SCCDFTB level and refining the potential at the DFT level.

The resulting DNNPs accurately reproduce both intra- and intermolecular properties of water clusters in excellent agreement with reference calculations, thus enabling reliable simulations at a drastically reduced computational cost. This approach allows, for the first time, the computation of heat capacity curves for large water clusters at the DFT level of accuracy including NQE. It opens the way to a detailed, quantum-level understanding of finite-size effects and phase transition behaviors in water clusters previously inaccessible due to computational limitations.

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Molecular Investigation of the Interaction of Fluorescent Probes with Early Protein Aggregates

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Introduction. We recently proposed a trap-and-release tandem ion mobility method to monitor the temperature-dependent kinetics of conformational changes in biomolecules. We demonstrated a proof-of-concept of this method on the model peptide (1). Using these techniques, we will investigate the connection between fibril morphology of protein aggregation and its binding ability with a fluorescent chromophore used in detecting these fibrils. We shall use the yeast prion protein Sup35 (aggregate forming peptide) and thioflavin T (chromophore) as our model.
Methods. We use a homebuilt dual drift tube instrument coupled to a time-of-flight mass spectrometer. This unique setup allows for the selection of an isomer or a conformer in the first drift tube. The selected ions are then stored in a thermalized RF ion trap for a controlled duration. Finally, the second drift tube allows to monitor possible conformational changes.
Results. Results on the conformation and kinetics of small oligomers of a short peptide sequence of the yeast prion protein Sup35, which is known as a model for amyloid fibril formation (2), will be shown.
Impact. Beyond the above-cited relatively small molecular species, the proposed method may be of interest to larger systems, especially β-amyloids fibrils. The present work paves the way to such applications.

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O14

Biomass conversion to added value products under Visible light excitation of Metal Halide Perovskites supported hollow spheres

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The selective conversion of biomass-derived molecules into high-value chemicals under mild conditions remains a key challenge in green chemistry. In this study, we report a highly efficient photocatalytic system consisting of $CsPbBr_3$ perovskite supported in hollow spheres of titanium dioxide (TiO_2). The designed architecture promotes strong light absorption, efficient charge separation, and enhanced stability of the perovskite under reaction conditions. Under visible light irradiation, the hybrid catalyst enables the selective oxidation of 5hydroxymethylfurfural (HMF) to both 2,5-diformylfuran (DFF) and 2,5-furandicarboxylic acid (FDCA), two major platform chemicals to produce bio-derived polymers. Mechanistic studies reveal that the synergistic interaction between the $CsPbBr_3$ and TiO_2 facilitates the generation of reactive oxygen species and directs the oxidation pathway. This work demonstrates a powerful strategy for integrating halide perovskites into functional photocatalytic systems for sustainable biomass enhancement under visible light.

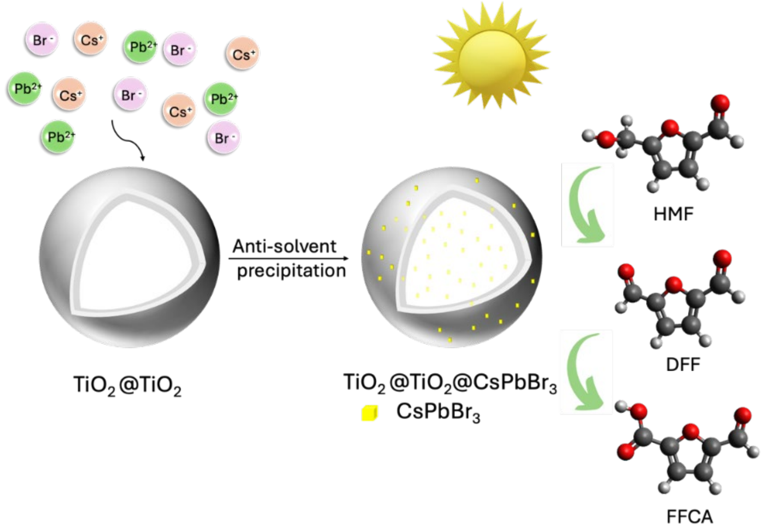

Figure: Schematic illustration of the photocatalytic oxidation of 5-hydroxymethylfurfural (HMF) to 2,5diformylfuran (DFF) and 2,5-furandicarboxylic acid (FDCA) using a $TiO_2@TiO_2@CsPbBr_3$ hollow spheres catalyst under visible light irradiation.

O15

Elucidating the complex photophysics of luminescent donor-acceptor keto-coumarins

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Luminescent donor-acceptor organic molecules are popular in various fields of applications, such as flexible displays or sensors. They provide various and complex radiative deactivation pathways that can be fine-tuned through molecular design. In the solid state the optical properties can also be altered significantly depending on the preparation method, which has important implications in device fabrication. In certain compounds, their emission spectrum is also subject to change when mechanical stress is applied, and this phenomenon is known as mechanofluorochromism. In this study, we explore long-lived emissive chromophores by studying the properties of two keto-coumarin derivatives with different donor groups (ECBP and DCBP, Fig. 1a).(1) Both compounds exhibit mechanofluorochromism, as well as long-lived emission. The degree of charge-transfer character is enhanced in DCBP due to the stronger diphenylamine donor, imbuing it with a greater degree of environmental sensitivity. Through a combination of time-resolved emission spectra, time-correlated single photon counting decay curves, steady-state spectra, quantum chemical calculations, and crystal structure analysis, the complex excited state dynamics can be deduced, resulting in a complete picture of the solid-state photophysics for these compounds. Remarkably, DCBP crystals decay via multiple radiative pathways, exhibiting dual prompt emission, delayed fluorescence and room-temperature phosphorescence (Fig. 1b).(2) Such compounds are extremely promising as emissive components in mechanosensors, biosensors/imaging agents, and information encryption.

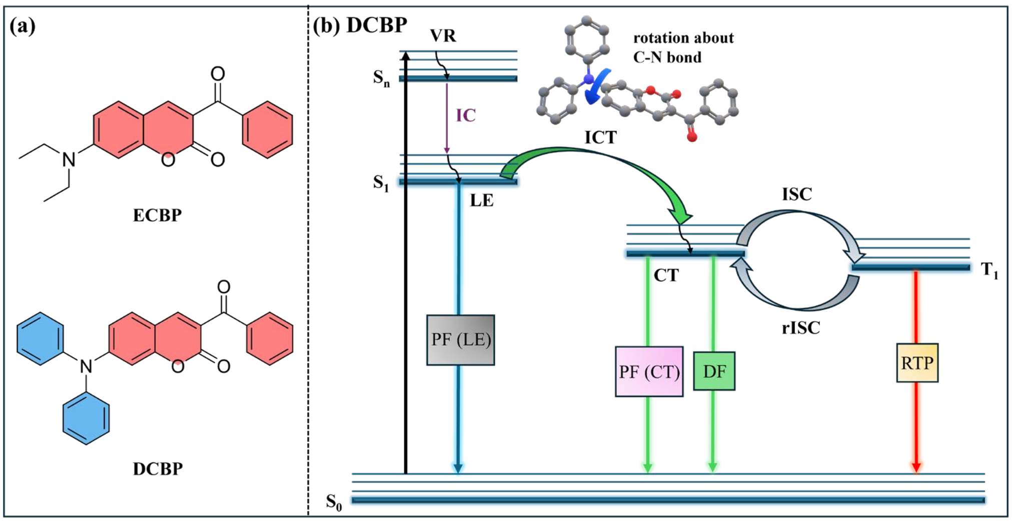

Figure 1: (a) Molecular structures of keto-coumarins ECBP and DCBP; (b) Perrin-Jablonski diagram representing excitation and the various decay pathways for DCBP crystals. VR – vibrational relaxation, IC – internal conversion, LE – locally excited state, CT – charge-transfer state, PF(LE) – prompt fluorescence from a LE state, PF(CT) – prompt fluorescence from a CT state, DF – delayed fluorescence, ICT – intramolecular charge-transfer, ISC – intersystem crossing, rISC – reverse intersystem crossing, and RTP – room temperature phosphorescence.

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Experimental study on the uptake of gaseous molecular iodine by atmospheric droplets

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Halogen compounds which are emitted from both natural and anthropogenic sources are well known as stratospheric ozone-depleting trace gases as observed during field campaigns or predicted by atmospheric models. Iodine species are highly reactive and can interact with the other atmospheric constituents (gas or particles) leading to its transformation into gaseous or particulate form. Moreover, iodine chemistry is an important driver of new particle formation in the marine and polar boundary layers [1, 2, 3]. The mechanisms governing the gas to particle conversion and the interactions between iodinated species and atmospheric pre-existing particles remain poorly understood.

The fate of the iodinated species has also a crucial interest in the field of nuclear safety. In case of a nuclear accident, radioactive iodine e.g., ^{131}I will be released to the atmosphere and can cause adverse health effects when inhaled or ingested [4]. It is therefore essential to understand its reactivity in order to improve predictive atmospheric dispersion models and take appropriate measures to protect populations. Addressing this gap is the main objective of the ASNR SPECIOSA program to which this study will contribute. One of the first gas to particle conversion processes is the absorption of the gas phase by the aqueous droplet, described by the solubilization of gas in solution, i.e. Henry's law. However, a significant gap exists in experimental data on gaseous molecular iodine (I_2) uptake by aqueous atmospheric particles. Such data are important for refining the radioiodine dispersion modeling tool used in the event of a nuclear emergency. In this context, this work aims to contribute to the understanding of atmospheric iodine chemistry through experimental approaches by focusing on inorganic iodine-aqueous phase interaction.

Here, we investigated the uptake of I_2 by aqueous droplets models of atmospheric particles, using an experimental setup based on the droplet train technique. This experimental set up is a widely used method for studying gas-liquid interactions [5, 6]. The set up has been built, optimized and validated to perform uptake experiments under near-atmospheric conditions. The first uptake experiments were performed with pure water droplets of diameter ranging from 100-200 µm. Dependence of the uptake coefficient on the gas-liquid contact time and droplet composition was also investigated. Analytical techniques such as ICP-MS were employed for the analysis of the liquid phase (collected droplets) and UV-Vis Spectroscopy was used for the quantification of the gas phase captured in a trapping solution. The strength and limitations of the experimental set up for measuring the uptake coefficient were also explored and will be presented.

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Raman Optical Activity and ECD-Raman in Chiral Transition Metal Complexes

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Raman Optical Activity (ROA) is the differential inelastic scattering of left and right circularly polarized light by a chiral medium [1]. ROA, combined with computational calculations, provides numerous spectral bands, giving details on structure, geometry and absolute configuration of system [2]. Even though ROA has been used for the detailed structural analysis ranging from simple organic molecules to proteins and viruses [3], it is relatively a young candidate in the characterization of coordination metal complexes [4].

Chiral coordination complexes attract attention due to their plethora of applications, ranging from asymmetric catalysis to medicinal properties, and due to the tunability of their molecular structures resulting from the variety of coordination numbers and multiple means to introduce chirality [4]. This work focuses on the comparative study of experimental and theoretical ROA results obtained for chiral diamine-based first row transition metal complexes. Additionally, for these compounds, we measure the intense signals of ECD-Raman, a recently discovered spectroscopy [5], which arises from the interference of Electronic Circular Dichroism (ECD) of the chiral solute and Circularly Polarized Raman (CP-Raman) of both achiral solvent and solute, in systems in or near-resonance.

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Tautomerism and Conformational Effects in Protonated and Copper(I)-Coordinated Bis(oxazoline) Ligands: Insights from IRMPD Spectroscopy and DFT

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Tautomerization and conformational flexibility play a central role in shaping the structure and reactivity of bis(oxazoline) (BOX) ligands, both in their free protonated forms and when coordinated to metals. We present a combined spectroscopic and computational study of (S,S-Ph-BOX)H^+, its dimethylated analogue (S,S-Ph-diMeBOX)H^+, and their corresponding copper(I) complexes. IRMPD spectroscopy and ion mobility measurements, supported by DFT calculations, reveal tautomerism in the protonated (S,S-Ph-BOX)H^+ and a broader conformational ensemble in the sterically constrained diMeBOX derivative. For copper(I)BOX complexes, large variations in calculated ligand dissociation energies (BDEs) are traced to the choice of conformer and tautomer. Comparison with experimental IRMPD spectra confirms that only the correct tautomeric form yields reliable agreement with measured BDEs. These findings underscore the importance of tautomer control for accurate structureenergy relationships in BOX-based catalytic systems.

O19

Modeling the Vibrational Circular Dichroism spectroscopy of Phenylcyclohexanediol and Ionic Liquids to probe solvation properties

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Vibrational circular dichroism (VCD) unveils molecular conformational nuances by discerning absorption differences in right- and left-circularly polarized light within the infrared range (1). This subtle technique elucidates molecular interactions, especially those that are sensitive to hydrogen bonding, thereby offering particular insight into the structure of unconventional solvents. Interpreting VCD signals necessitates meticulous comparison with theoretical models. However, incorporating environmental effects posed challenges, now mitigated by advancements in computational modeling. Recently, we proposed a new methodology (2) based on classical molecular dynamics simulations associated with the AMOEBA polarizable force field (3) to calculate VCD spectra of flexible molecules. The crucial element in these VCD simulations is determining the magnetic dipole moment, an intrinsic dynamical quantity. Highly flexible molecules, ionic liquids (ILs) and deep eutectic solvent (DES) turn out to be particularly interesting to study with this methodology. The 1-phenyl1,2-cyclohexanediol (PC), a highly flexible molecule, was successfully studied in dimethyl sulfoxide (DMSO) solvent, by calculating both infrared and VCD spectra and the comparison with experimental data. Furthermore, these spectra were calculated for ILs and DES, to probe their long-range organization which appears challenging, especially for VCD spectra. In particular a studied was made on spirocyclic pyrrolidinium tetrafluoroborate and menthol acetic acid respectively. Modeling both the infrared and VCD spectra for these systems reveals useful microscopic-scale information on solvation at the molecular level.

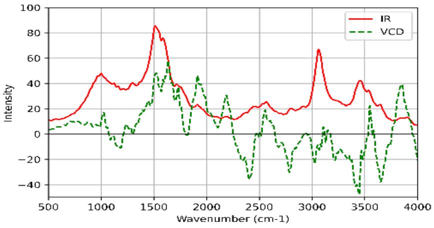

Figure: *Infrared and VCD spectra of PC in a box of solvent (DMSO)*

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O20

Advanced modelling of nonlinear optoelectronic properties of functionalized CdTe quantum dots using machine learning combined with DFT

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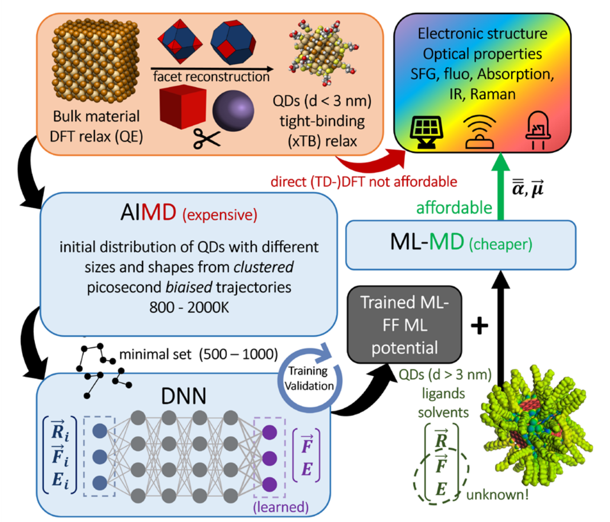

Figure: Graphical abstract. Modelling QDs properties using DFT combined with deep potentials.

Zinc-blende CdTe quantum dots (QDs) exhibit unique electronic structure and optical properties with applications in the realm of photovoltaics (QDSSCs), optoelectronics (QLEDs), biomedicine (biosensors, biolabeling). A high tunability of their optical properties (quantum yield, optical gap) can be achieved by varying their size, structure, and capping ligands. Thus, a proper modelling of their surface chemistry is necessary to allow for both their stability and quantum confinement of the electron-hole states [1]. Advances in the synthesis of QDs—including growth pathways for the nanocrystalline core and innovative methods to control their surface functionalization [2]—report magic-sized QDs which exhibit enhanced stability and quantum properties for specific ligands. Yet only the optoelectronic properties of small capped-clusters (d<2nm)— below the experimental relevant range (d=3-10nm)—can be theoretically studied through the framework of density functional theory (DFT) and its time-dependent counterpart (TD-DFT) due to exponential computational costs. This work aims at bridging this gap by developing a machine-learning approach to design and study large QDs with DFT-level accuracy at a low computational cost. Deep Neural Networks (DNN) algorithms, such as DeepMD, have been shown to be efficient in the construction of machine-learning force fields for system of higher dimensionality down to small PbS/CdSe QDs ($\lesssim$ 1000 atoms) [3], [4]. Nevertheless, they require a comprehensive dataset, of reasonable size that accurately encapsulates the relationship between a QD's size, structure, surface passivation, and the corresponding atomic energies and forces. We propose an initial dataset comprises DFT characterized Cd_nTe_m structures (n = 13–119, m = 16–119) with passivated and geometrically relaxed surfaces. We consider active learning to gradually scale the range of structures in order to allow model generalization. Once validated, the model will be used to compute Sum Frequency Generation (SFG) spectra [2], [5] via molecular dynamics simulations to probe ligands-QDs surface interactions. These nonlinear optical properties rely on the full polarisability tensor and remain largely unexplored by the existing literature.

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Production and study of model nanoplastics by top-down and bottom-up methods for environmentally relevant studies

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Although nanoplastic pollution is today a threat, most toxicological studies published so far use commercial polymer latexes i.e. perfect cross-linked polystyrene nanospheres modified by surface moieties, e.g. carboxylate groups. In fact, PS-NPs have little to do with real nanoplastics found in environment, of irregular sizes and shapes due to physical wearing, bearing UV-oxidized surface, coated by organic and biological layer (humic acids, ”plastisphere”...). The latest literature reports two types of reference materials for environmentally relevant nanoplastics for collaborative research with (eco)toxicology laboratories:

Type A NPs suspensions produced by top-down method initially described by El Hadri et al. (1), i.e. by crushing plastics litter collected by citizen associations from seashore or riverbanks. Such type A NPs are considered as “environmental nanoplastics” more representative of naturally occurring NPs (Env-NPs) produced by plastic weathering (by sun light, abrasion...) than PS-NPs.

Type B NPs prepared in the lab by bottom-up assembly of polymer chains. Briefly, virgin plastic pellets first dissolved in an organic solvent miscible with water are mixed with an excess of water acting as bad solvent. This so-called “nanoprecipitation” method can reach high solid content (up to 1 wt%) and control of particle shape and size-distribution.

First results of ecotoxicological assays on aquatic organisms (algae, clams and oysters) show that Type A NPs exert stronger impacts than Type B NPs , made from either petro- or bio-sourced polymers: even sublethal concentrations (10-100 µg/L) lead to inflammation in the organisms (2), which might arise because synthetic Type B NPs are chemically pure compared to Type A Env-NPs made from plastics weathered for decades, containing various dopants or contaminants.

The main pitfall to introduce a regulatory framework in assessment of nanoplastics is the lower limit of detection of the analytical methods, for their quantification and identification. Progress has made it possible to detect NPs in pure water (using for example pyrolysis-GC/MS technique) or in aerosols, but the next steps would be to identify and quantify them in complex matrices (soils, sea or fresh water, living tissues...). Like any colloids, dynamic light scattering (DLS) is recommended to follow the dispersion state of NPs in water. The hydrodynamic size of NPs measured by DLS

generally ranges from 100 to 500 nm. The size distributions can be monitored and, to some extent, controlled by physicochemical means (e.g. size fractionation by ultra-centrifugation).

In true ecological samples (at high dilutions), it is recommended to choose a DLS instrument with variable scattering angle (goniometer) rather than a fixed angle (usually 90◦ or 173◦) to benefit from the angular form factor of particles, as explained in reference (3). The authors mention a LOD of 1 µg/L using a very low scattering angle (belon 20◦) but in practice, the detection limit that we found with such small angle DLS is more likely around 10 µg/L. This technique enables us to study the colloidal stability of Type A or Type B model NPs when exposed to high ionic strength sea water, through a microfluidic mixing chamber that mimics the slow mixing conditions in natural river estuaries like in Arcachon basin (4). One way to decrease the LOD of nanoplastics could be to label them with metals (Fe, Au...) that can be traced at very low concentration (nM) thanks to their either magnetic (Fe) or optical (Au) “fingerprints”: Au-labelled NPs would be possible to detect in complex media and to differentiate from other organic matter by SERS spectroscopy or imaging.

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Accelerating the Structure Exploration of Diverse Bi–Pt Nanoclusters via Physics-Informed Machine Learning Potential and Particle Swarm Optimization

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Bimetallic nanoparticles (NPs) have received tremendous interest in the fields of catalysis, energy materials and biomedical applications, thanks to their synergistic interactions between their constituents. Our interest lies particularly in the Bi-Pt system, shown, for exemple, to have enhanced catalytic activity over the simple Pt catalyst in the electrooxydation of formic acid[1], have been employed to monitor temperatures in reactor melt wires and have been synthesied as radio-enhancers for radiotherapy[2].

Theoretical investigations of this system are rare and difficult to realize. The potential energy landscape of such a system is vast and complex, notably due to the mixing of two elements with differing crystal structures (rhombohedral bismuth and cubic face centered platinum) and the abundance of structural variety emerging from it (Core-shells, Janus and other alloy configurations). Thus, we employ machine learned interatomic potentials (MlIPs), trained on DFT level data to maintain accuracy, while significantly improving calculations costs. In our work, we focused on the the Chebyshev Interaction Model for Efficient Simulation (ChIMES)[3], a physically informed ML potential based on multibody interaction cluster expansion and Chebyshev polynomials. We successfully trained the model on the data scarce system, iteratively improving and growing our training data via active learning. Once capable of delivering accurate predictions of energies and forces, we paired the ChIMES model with a global optimisation algorithm, CALYPSO[4] leveraging its exploratory capabilities for an efficient simulation of the system's structural space.

Finally, we exploited all the data accumulated on the system, including spectral properties (IR, DOS and VDOS), structural and shape descriptors (e.g coordination numbers, radial distances...) and electronic properties (e.g cohesion energy, band gap...) to obtain a machineled classification of the structural types observed. This data led approach, via principal component analysis and k-mean clustering, is compared with a manual classification of the structures obtained into Core-shells, Janus and mixed alloys. These results and methods are further explained in an upcoming article[5]. We now aim to further understand the impact of data selection on our model training, compare its behavior and suitability with foundational models pretrained on large databases and to advance the study of the system, notably by including NPs with varying metallic ratios, sizes and potentially the chemical environment.

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Experimental Characterization and Theoretical Modelling of X-ray Absorption Spectra of Protactinium(V) Complexes

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Protactinium (Z = 91) exhibits unique redox behavior, oscillating between Pa(IV) (1) and Pa(V). In aqueous media, Pa(V) predominates as Pa5+ or PaO^{3+}, while $PaO2^{+}$, common in heavier actinides, has not been observed (2,3). The presence of a potential mono-oxo bond in Pa(V) can be investigated using X-ray spectroscopies (4).
In February 2024, HERFD-XANES, RIXS, and EXAFS experiments at the MARS beamline (SOLEIL) were performed to study Pa complexes. Unexpected, the spectra of PaV in oxalate and fluoride solutions showed strong similarity challenging earlier interpretations suggesting mono-oxo formation in oxalic media (5). To interpret these findings, we employed relativistic TD-DFT (6) and RASSCF (7) simulations at the L3 and M4 edges using EXAFS-derived structural models. These theoretical approaches not only accurately reproduced the experimental spectra but also provided insights into the nature of the electronic transitions.

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Electrochemical Analysis by mass spectrometry to study furfural reduction reactivity

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Understanding of the reactions in an electrochemical reactor is mandatory to develop more efficient catalysts. Mass spectrometry is a versatile tool that can give access to interesting information on the formation of final products, intermediates and subproducts. However, the association of the two techniques is limited due to the electrochemical medium which combines high concentrations and strong electrolytes.

We target a reaction from the transformation of the biomass. The depolymerization process leads to the formation of oxygenated monomers that needs to be reduced to be used in another chemical processes. We study then furfural reduction to 2-methylfuran in an acidic media.

Solutions are studied in a Q-TOF (6600 Sciex) with a dualspray (APCI and ESI). First, solution parameters (pH, salts, concentrations) are tested to identify the optimum conditions to obtain a response for the targeted molecules. Secondly, a flowcell is adapted to the instrument using the optimal conditions defined previously. Lastly, we developed a DEMS to study at the same time the gases and small molecules formed in the solution.

We present the results of the experiment. Optimal conditions are obtained after dilution in a MeOH/H_2O solvant. The species studied (FF, 2MF and FOH) presents a linear response. We could study the solution in a flow cell adapted for the dilution before analysis.

O25

Electrostatically Embedded QM/MM Study of the Potential-Dependent Reorientation of Pyridine on Au(111)

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Electrified interfaces are the key to heterogeneous electrocatalysis. To achieve an atomistic description of the reactivity, grand-canonical density functional theory (GC-DFT) is one of the most popular and convenient approaches. However, the accuracy of the widely used implicit solvation models, that are usually used in combination with GC-DFT, is questionable. We have developed a quantum mechanics (QM)/molecular mechanics (MM) approach, applied to surfaces and solvent, respectively, to model the solvent in a more realistic way without significantly increasing the computational cost.[1] First, GC-DFT with an implicit solvent is employed to establish the geometry and the atomic charges. This information is then used for explicit solvent molecules and electrolyte MM-based molecular dynamics (MD). The average charge distribution from MD is extracted and combined with GC-DFT. In this work, the hybrid QM/MM scheme with electrostatic embedding is applied to a system where the water solvent interacts with moderate strength with the metallic gold electrode: the potential-dependent reorientation of pyridine adsorbed on Au(111), which is experimentally well characterized. Three coordination modes of pyridine to Au surface have been reported: parallel adsorption of the aromatic ring, tilted and perpendicular adsorption via lone-pair electrons of the N atom.[2] For each mode, the grand-canonical adsorption energy has been evaluated as a function of potential and coverage to determine the most favorable one as a function of the potential. In contrast to implicit solvents[3], the transition potential is predicted in reasonable agreement with experiment, see Figure 1. Our benchmarking study shows that both the precise nature of the solvent treatment and the choice of the density functional approximation has large impacts on the predicted adsorption and reorientation potential. This suggests that pyridine on Au(111) is a very challenging test system as it exhibits a subtle competition between pyridine and water adsorption.

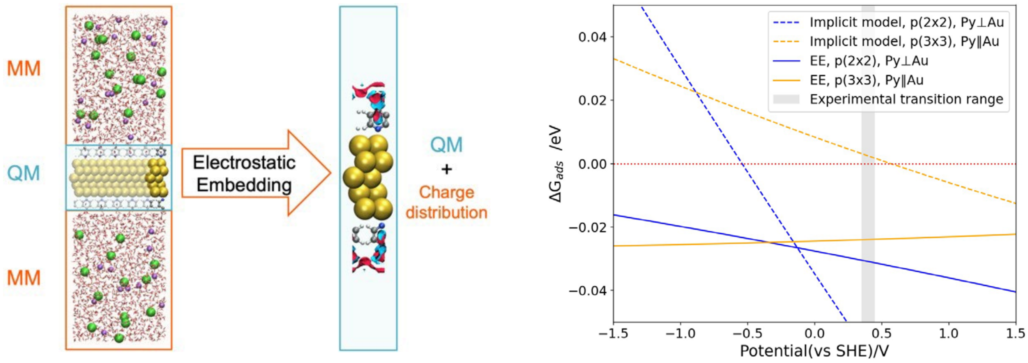

Figure: Left: Schematic picture of our QM/MM scheme. The charge distribution of the MM part is used to determine the electrostatically embedded (EE) QM energy. Right: Adsorption energy per Au surface atom as function of electrochemical potential. The transition potential obtained by EE (-0.4 V vs SHE) is more consistent than when using an implicit solvent (-0.9 V) compared to the experimental results of ref [2] (0.4 V).

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ICONE: une nouvelle source compacte de neutrons pour la physico-chimie.

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La communauté française des utilisateurs de la diffusion des neutrons compte plus d'un millier de membres, dont une large fraction de physico-chimistes. A la demande du CEA et du CNRS, le Laboratoire Léon Brillouin - au nom de la communauté française - développe le projet d'une nouvelle source de neutrons ambitieuse, basée sur le concept innovant dit HiCANS (*High-Current Accelerator-based Neutron Source*). ICONE, pour *Innovative Compact NEutron source*, est une infrastructure visant à doter la France d'instruments de diffusion des neutrons aux performances équivalentes ou supérieures à celles disponibles sur les sources nationales existantes en Europe, avec un accès simplifié et rapide. En offrant des instruments performants de diffraction, de diffusion aux petits angles, de spectroscopie, d'imagerie, d'analyse élémentaire et des lignes multi-techniques, la suite instrumentale envisagée répond aux points forts de la communauté française dans le domaine des sciences moléculaires, de la matière molle et des systèmes complexes allant de la biologie aux macromolécules et nanostructures; dans le domaine des matériaux innovants allant de leur chimie au magnétisme en passant par le quantique; ou encore dans le domaine des applications finalisées tels que les géosciences, le climat, l'environnement ou le patrimoine, et de l'industrie pour les grands secteurs tels que l'énergie, la santé ou les nouvelles technologies du numérique – avec un atout fort de l'installation lié à sa flexibilité et à son mode d'accès rapide.

Cette source offrira ainsi à la communauté française la capacité de réaliser toutes les expériences nécessaires aux recherches allant de la physique à la chimie en passant par la biologie, afin d'acquérir les connaissances et le savoir-faire en diffusion des neutrons et ainsi d'accéder aux sources de très haute brillance comme ESS (European Spallation Source) en Suède ou actuellement, l'ILL (Institut Laue Langevin) à Grenoble.

Cette présentation développera les concepts originaux mis en place pour une telle source de neutron tant au niveau de la production des neutrons, de l'instrumentation que du modèle d'accès. Un point particulier sera porté sur les apports d'ICONE pour la communauté des physico-chimistes, grâce à la suite instrumentale unique permettant des études de structure sur de grandes échelles spatiales et des études de spectroscopie sur des échelles de temps donnant accès aux relaxations et excitations dans la matière.

Fluids at an electrostatically active surface: Optimum in interfacial friction and hydroelectronic drag

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Fluids at solid interfaces are central to key technologies in energy conversion, electrochemistry, and catalysis, yet their nanoscale dynamics remain only partially understood. On metallic surfaces, recent studies have revealed unconventional interfacial phenomenaincluding complex electrostatic screening, anomalous wetting behavior, and quantum frictionthat call for new modeling tools bridging charge dynamics in the metal with molecular motion in the fluid. In this talk, I will introduce a molecular simulation framework based on Virtual Thomas-Fermi fluids, enabling a realistic, atomically-resolved treatment of interfacial transport that captures both charge relaxation in the metal and its coupling to the surrounding liquid. Applying this approach to water near metallic surfaces with tunable screening properties, I will uncover a non-monotonic dependence of interfacial friction on metallicity, peaking when charge relaxation modes in the solid and fluid dynamically overlap. Furthermore, I will show a direct observation of hydroelectronic drag, a momentum transfer mechanism rooted in dynamic electrostatic interactions at the interface. These results shed new light on interfacial transport under electrostatic coupling and open avenues for designing metal–fluid interfaces with tailored frictional properties.

O28

Impact of the Host Polymer Viscoelastic properties on Magnetic Hyperthermia of Nanocomposites

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Magnetic hyperthermia arises from heat dissipation by magnetic nanoparticles (MNPs) exposed to an oscillating magnetic field (OMF). This phenomenon has garnered significant attention due to its promising applications in biomedical engineering, materials science, and chemistry.(1) While heat generation is often associated with magnetic hysteresis losses, which are primarily determined by the intrinsic properties of the nanoparticles, our recent findings highlight the crucial role of the surrounding medium.(2)

In this work, we embedded iron oxide nanoparticles in polypropylene, a phase transition polymer, of various viscosities ($0.70 < \eta 0 < 9400$ Pa s) and investigated the role of the host polymer viscoelastic properties and its influence on the heating efficiency of the MNPs.

We demonstrate that the reorganization of the NPs into dipolar columns tends to enhance the global specific absorption rate (SAR in W g^{-1}) of the nanocomposites. The SAR, which describes the amount of energy converted into heat per gram of magnetic content, is commonly determined from the initial slope of the heating curves. As illustrated in the figure 1, the initial rise of temperature of the first heating curve is less steep than the second and third heating curves. 2D SAXS pattern revealed that once the melting point of polypropylene is reached, the initially isotropic pattern becomes anisotropic. These findings have been supported by microscopy images in which we can see NPs organized into dipolar chains after the first heating. In addition, by exposing the nanocomposites under an OMF and probing their structure *in-situ* with X-ray Photon Correlation Spectroscopy (XPCS), we also investigate how the dynamic of MNPs rearrangement into dipolar columns is impacted by the host polymer viscosity. Overall, our study highlights the multiple heating mechanisms involved in magnetic hyperthermia - magnetic hysteresis, MNPs reorganisation and friction between the MNPs and its surrounding - with the aim of corroborating computational models (3,4) with new experimental insights.

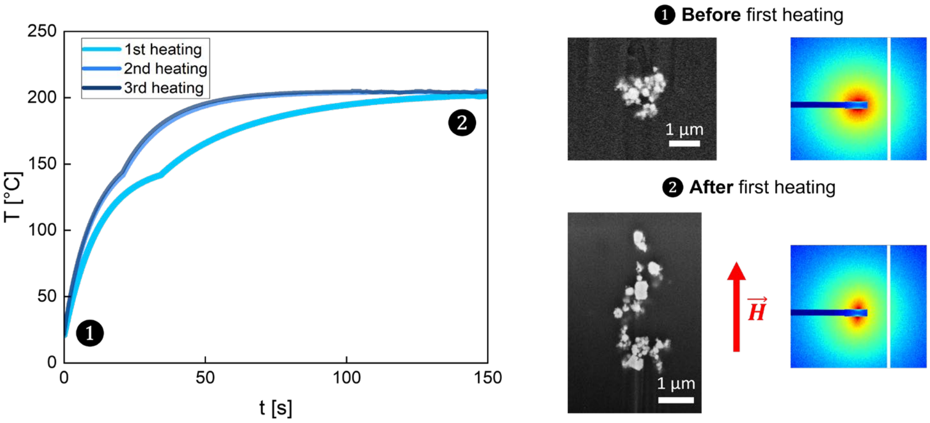

Figure 1: (Left) Temperature evolution of a polypropylene-Fe_3O_4 nanocomposites under a high frequency oscillating magnetic field. (Right) Scanning Electron Micrographs and 2D SAXS pattern of as-made nanocomposite (step 1) and irradiated nanocomposites (step 2). The red arrow indicates the direction of the applied magnetic field.

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Excited-state dynamics and thermal recovery of salicylidene-aniline photoswitches: a theoretical investigation

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Photo-induced reactions in molecules are key to developing novel light-responsive systems and applications. One particularly interesting group of molecules are photochromes, which reversibly switch between two metastable forms upon irradiation. These light-controlled "molecular switches" or *photoswitches* hold potential for many applications, such as: photocontrollable materials, photo-pharmacology, and solar thermal energy storage.[1] Understanding photoinduced processes in these molecules, through a combination of theory and experiment, can enable intelligent selection and design of improved photoswitches.

In this contribution, I will present our theoretical study of the salicylidene aniline (SA) photoswitch, which upon UV irradiation (355 nm) undergoes an ultrafast excited-state intramolecular proton transfer (ESIPT), followed by photoisomerisation to form the metastable *photochromic* form.[2] I will highlight two key aspects of our investigations. First, I will discuss the initial sub-100 fs ESIPT reaction, which we model with mixed quantum classical non-adiabatic dynamics simulations. In particular, I will highlight the importance of an accurate preparation of the initial molecular wavepacket. Second, I will discuss the thermal recovery pathway which leads to reformation of the initial molecule from the *switched* form, which we demonstrate through combined theory and experiment to take place through a solvent-assisted mechanism in a "protonated" form, challenging previous assumptions made in literature.[3]

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Theory and Lattice Boltzmann Modeling of Complex Pollutants in Solution: Effect of the Porous Medium Heterogeneity on Adsorption and Transport

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In recent years, a strong interest was shown by the large public for the impact and fate of new pollutants which are threatening the environment as well as human health [1]. Consequently, in parallel to recent technical progress, large efforts in fundamental and applied research were devoted to this field. Many detection and remediation tools have been developed in the past years for emerging pollutants such as per- and polyfluoroalkyl substances (PFAS), pharmaceutical and personal care products (PPCP), antibiotics, etc. In addition to the role of numerous environmental parameters (pH, salinity, coexisting organic matter, ions, etc.), the chemical (*e.g.*, composition, molecular structure, dissociation) and physical (*e.g.*, phase diagram, solubility, aggregation) specificities of these complex molecules lead to a rich and intriguing behavior near solid surfaces [2,3]. In this context, while adsorption-based solutions offer promising perspectives for efficient remediation approaches, their development is limited by significant knowledge gaps in the fundamental mechanisms governing the behavior of emerging pollutants in solution and near solid surfaces. By adopting a fundamental physical chemistry perspective, we develop a robust model that includes the effects of surface saturation, reservoir depletion, and lateral interactions on the adsorption kinetics and thermodynamics of PFAS molecules. More specifically, a thermodynamic framework that accounts for two- and three-body lateral interactions is built and the effect of each interaction parameter on the shape of the adsorption isotherm is investigated. Then, a thorough kinetic model based on the thermodynamics of adsorption and on a rigorous definition for the adsorption and desorption rates (which, in a general framework, should include surface saturation, reservoir depletion and lateral interactions) is developed. The latter is then implemented into Lattice Boltzmann simulations to numerically solve the transport equations governing the mass transfer of complex pollutants in bimodal porous media [4, 5]. These media serve as simplified yet effective representations of natural media such as soils or sediments as well as adsorption-based filtration systems. Our approach aims to characterize both the effects of dual porosity and topological heterogeneities of the media on the adsorption and transport mechanisms of emerging contaminants such as PFAS. Our approach provides new insights into the interplay between adsorption and transport mechanisms in heterogeneous media. As a long-term perspective, the present work could pave the way for improved remediation strategies using porous filters and provide a deeper understanding of the impact of emerging pollutants on natural porous environments (*e.g.*, soils, sediments).

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O31

Interplay of Structure and Dynamics in Solid Polymer Electrolytes: a Molecular Dynamics Study on poly(propylene carbonate)-based / lithium salt

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Solid-state batteries (SSBs) are emerging as the next major advancement in electrochemical energy storage devices [1]. Compared to conventional liquid Li-ion batteries, SSBs offer higher energy density with the use of the Li metal as negative electrode and the enhanced safety with the suppression of flammable liquid electrolyte [2]. To improve the transport properties in SPEs, it is crucial to understand the interplay between the structural and the dynamic properties in the bulk and under confinement in the electrode pores.

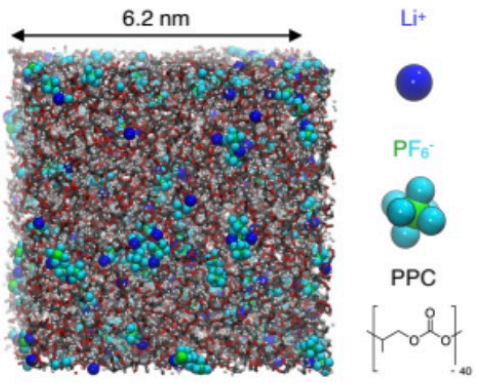

Figure: Typical configuration of the molecular model of $LiPF_6$-poly(propylene carbonate) solid polymer electrolyte at 1.2 mol kg^{-1}

This study aims to provide a comprehensive understanding of the molecular mechanisms in poly(propylene carbonate)-$LiPF_6$ based SPEs using all-atom molecular dynamics with classical force fields from the literature [3]. The structural and dynamics properties of the SPEs have been studied at different salt concentrations (0.3 to 1.2 mol kg^{-1}). The results show a strong ionic association and the formation of ionic cluster which are mainly electronegative when the salt concentration increases. For dynamics properties, a small dependence on the salt concentration was observed. The model was extended to confined SPE between lithium cobalt oxyde surfaces to study the electrolyte ordering near and far from the surface and the impact on transport properties.

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O32

Microscopic view of hydrogen adsorption in size-variant nano-clays materials

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Hydrogen is the carbon-free fuel par excellence because its combustion emits only water. Research has focused on H_2 storage in lightweight materials for the needs of vehicles, excluding clays due to their weight. But large-scale terrestrial storage for industrial applications does not require the same specifications. In this context, clay minerals offer several interesting properties, such as large surface area, low cost, global abundance, and environmental safety.

We investigate, at the microscopic level, H_2 adsorption on synthetic 2:1 trioctahedral smectites of nanometric dimensions, specifically Laponite, and its precursor, pre-Laponite. Our aim is to understand the higher H_2 sorption capacity of pre-Laponite, combining adsorption isotherm measurements, elastic and inelastic neutron scattering experiments and Grand Canonical Monte Carlo (GCMC) simulations.

The adsorption isotherms at 40 K, up to 1 bar, are fitted with a Langmuir contribution and a smoothest one. GCMC simulations show that the Langmuir model, accounting for the strongest binding sites, describes adsorption within the interlayer, as confirmed by small angle neutron scattering. Inelastic neutron scattering experiments were undertaken to probe the para-to-ortho rotational transition of H_2, the energy of which is highly sensitive to its environment. At 40K, two adsorption sites are identified in the interlayer, with orientational potential wells of about 80K and 1300K, respectively. Based on wide angle neutron scattering analysis, the second site would be situated above the hexagonal cavity defined by Si tetrahedra. Quantum sieving effects were also evidenced comparing D_2 and H_2 adsorption. The highest adsorption in pre-Laponite compared to Laponite is attributed to the slightly more open interlayer space (sheet-to-sheet distance is 1 nm in pre-Laponite and 0.97 nm in Laponite).

The perspective of these results is the fine modulation of the interlayer space to optimize the storage of hydrogen in clays at low temperature and beyond, under pressure, at room temperature.

O33

Quantum algorithms for excited-state chemistry

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Quantum physics and chemistry have provided well-recognized theoretical tools to predict the behavior of molecules and materials described by the Schrödinger equation. However, many problems with high industrial and societal impact remain intractable for classical computers, urging us to reconsider our preconceptions and shift gears. The world of the infinitely small obeys the laws of quantum mechanics, suggesting the need for a machine governed by the same physics: this marks the birth of quantum computers, a new technological revolution which promises a quantum advantage (speed-up) over classical computers. In this talk, I will present the state-averaged orbital-optimized variational quantum eigensolver (SA-OO-VQE), designed to address the electronic structure problem for excited states (13), essential to unravel ubiquitous ultrafast (subpicosecond) photochemical and photophysical 'energy/charge/matter/information'-transfer processes induced upon the absorption of light by molecules within the UV-visible domain. I will show that SA-OO-VQE exhibits a propensity to produce an ab initio quasidiabatic representation "for free" if considered as a least-transformed block-diagonalization procedure (4). These recent findings underscore the practical utility and potential of SA-OO-VQE for addressing systems with complex nonadiabatic phenomena.

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POSTERS

P01

Dynamics and Interactions of Model Molecules with Porous Biomass-Derived Materials

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Porous carbon materials (PCMs), such as biochars derived from biomass, offer a sustainable approach to contaminant sequestration and environmental remediation. Their ability to interact with and immobilize organic molecules depends not only on the porous texture but also on surface chemistry. Although the adsorption properties of PCMs have been extensively studied, the molecular dynamics of confined solvents within their pore networks remain poorly understood.

In this study, we determined how model molecules having various size and polarity (H_2O, ethanol, toluene, and DMSO) interact and move inside the meso and/or microporosity of PCMs prepared with Sargassum from Guadeloupe island. To reach this goal, we probed the adsorption location of deuterated molecules using Small-Angle Neutron Scattering on D11 instrument at Institut Laue-Langevin (ILL, Grenoble, France). We also investigated the local dynamics of the same protonated molecules confined within PCMs using elastic fixed window scans (EFWS) on the IN13 backscattering spectrometer. Measurements were conducted during cooling from 300 K to 20 K to monitor temperature-dependent changes in elastic intensity, probing proton motions on the ~80 ps timescale. The evolution of elastic intensity with temperature offers a qualitative view of molecular mobility. From these data, quantitative mean square displacements ($\langle u^2 \rangle$) were extracted from linear fits of log I(Q) versus Q^2.

The combination of the results obtained with these two neutron instruments have shown that the mobility of molecules depends on their natures and their adsorption locations (meso or microporosity). This finding is very important for predicting the best PCMs/contaminant combination allowing an efficient sequestration.

Development and applications of AI based ab initio quality potentials for large clusters of astrophysical interest

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Although interstellar dust grains constitute only ~1% of the Milky Way's mass, they play a vital role in the physics and chemistry of the interstellar medium (ISM) [1]. The surfaces of these dust grains are coated with icy mantles. Ice mantles are mostly made of H_2O, CO, and CO_2 which are essential for shaping the chemical composition of interstellar gas clouds and reactivity [2]. Carbon monoxide (CO) is considered as the second most abundant molecule after molecular hydrogen (H_2) in interstellar space [3]. However, due to their low binding energies and complex potential energy surfaces (PES), theoretical research on compounds beyond CO dimers and trimers remains limited [4].

In this project, a systematic modeling of the homogeneous clusters of carbon monoxide $(CO)_n$ from small to large size was initiated by applying Deep Neural Network Potentials (DNNPs) trained with data generated from Parallel Tempering Molecular Dynamics (PTMD) simulations performed at the SCC-DFTB level using the deMonNano software package. Some of the generated structures are then subsequently re-optimized at the DFT level using a high-quality functional, ensuring accurate energies, forces for training the DNNP. The central obstacle is the development of a single transferable DNNP capable of accurately describing the PES across different cluster sizes once trained with DeepMD-kit software [5] where their accuracy and transferability are assessed across various cluster sizes. The primary goal is to obtain reliable structural ensembles of homogeneous CO clusters that will be analyzed and characterized. Future work will be expanded to mix water–CO clusters preparing insights into the structural evolution and interaction dynamics.

These advancements will contribute to a more realistic modeling of interstellar dust grains in terms of their size, composition, and dynamical processes such as growth, reactivity under astrophysical conditions.

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New heptazines derivatives: synthesis and photophysical properties

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Heptazine consists in the smallest triangulene doped with seven nitrogens distributed in an alternating pattern.[1] This peculiar structure confers a strong electron deficient character to this heterocycle along with precise repartition of frontier orbitals: HOMO is located on peripheral nitrogens whereas LUMO is on central nitrogen and carbon atoms. In terms of photophysical properties, this family of compounds is known to possess a small singlet-triplet energy gap, leading to delayed fluorescence properties. We have been particularly interested into a series of heptazines substituted by thiophenol derivatives, and we have been able to show that by tuning the electron-withdrawing or electron-donating character of the substituent on the thiophenol moiety (R group on figure 1) we can tune the fluorescence emission colour of the compound together with its delayed fluorescence properties. We will present the synthesis as well as the steady-state and time-resolved fluorescence properties of this series of compounds.

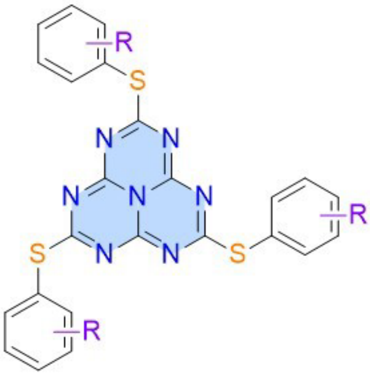

Figure 1: generic structure of heptazine substituted by thiophenols derivatives

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P04

Colloid self-assembling for the preparation of materials based on transition metals

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Porous materials have attracted significant attention in catalysis, adsorption, and drug delivery due to their high surface area and tunable pore structures[1]. In this study, we present a simple, environmentally friendly, and cost-effective method to fabricate oxide materials with an ordered inter-particular microporosity using a colloidal self-assembly approach in aqueous media[2].The synthesis relies on the controlled hydrolysis and condensation of metal precursors to tune the colloid size. Zirconium was selected as the initial metal due to its excellent thermal stability and wide applicability in catalytic and biomedical fields[3].

Zirconium colloids were synthesized using $ZrCl_4$ as a precursor at concentrations of 0.35 M and 1 M, maintaining fixed pH conditions at 1 and 10. Small-Angle X-ray Scattering (SAXS) analysis revealed colloidal aggregation at pH values between 3 and 10. At pH 1, charged ellipsoidal colloids with an average size of 1.6 nm were observed. The resulting sols were freeze-dried, and the scattering patterns of the obtained powder displayed a characteristic peak corresponding to a highly ordered arrangement of colloids with an average interparticle distance of approximately 1.2 nm almost similar to the ellipsoid size, regardless of the zirconium concentration. After thermal treatment at 300°C, scanning and transmission electron microscopy revealed that the powder consists of an assembly of ZrO_2 nanoparticles forming thin layers of few nanometers thickness. The presence of these nanometric layers indicates a high degree of homogeneity in the nanoparticle assembly. Further analysis of the SAXS data, based on Porod's law, the invariant theorem, and the Voronoi model, provided insights into several parameters: a specific surface area of approximately 100 m^2/g, a porosity of around 10%, and cylindrical pores with a length of about 16 nm and an inter-pore distance of approximately 1.6 nm.

These results highlight the potential of this aqueous colloidal method as a versatile and sustainable route for fabricating microporous oxide materials. Moreover, the method can be extended to incorporate other transition metals, allowing for further customization of material properties to meet specific applications

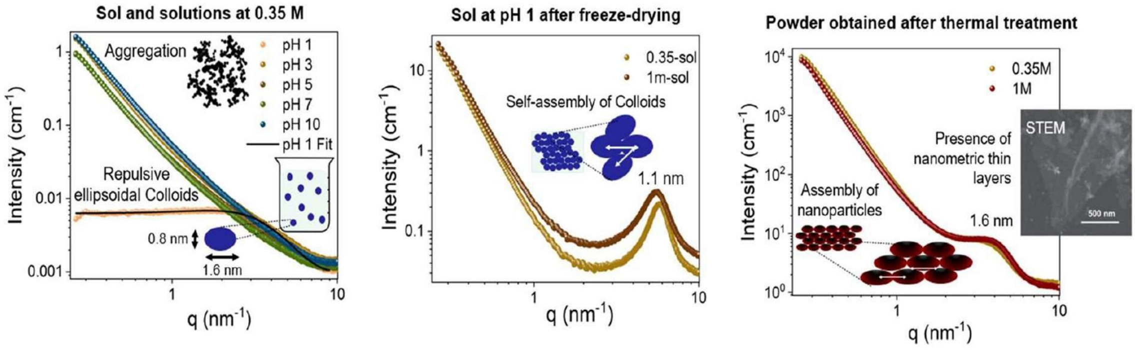

Figure 1: SAXS pattering of the solutions, the sols, the sols after freeze-drying and the powder obtained.

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Design and development of optical sensors for the detection of pesticide residues

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Although glyphosate is harmful to environment and classified as potentially carcinogenic to human health according to the International Agency for Research on Cancer (IARC), the assessment and quantification of this compound currently rely heavily on expensive and complex setups, such as: gas/liquid chromatography and mass spectrometry. In the EU, the maximum limit for most individual pesticides is established as 100 ng/L in drinking water. Our study aims to design and develop a sensitive optoelectronic sensor, enabling field measurements with a reasonably priced, portable system. In this communication, we will describe precise strategies for functionalizing gold nanoparticles surface using 4-thioacetate phenylacetylene as an anchoring ligand under in situ deprotection. This anchoring ligand type shows interesting results towards ligand's orientation on the surface depending on ligand quantity with two controllable distinct binding configurations, via Au-S and Au-C from terminal alkyne group, which we characterized by associating UV-Vis and Raman spectroscopy. In the future work, via “click” reaction, the free terminal alkyne of the anchoring ligand is then connected to azide modified CdSe quantum dots, providing gold nanoparticle – quantum dot hybrid nanosystem, allowing to detect the change in photoluminescence properties of the quantum dots or SERS of the gold nanoparticles in the presence of glyphosate. Ultmostly, success in our strategies will contribute to the development of a miniaturized analytical microdevice, targeting straightforward pesticide measurements, therefore promoting regulatory compliance in water supplies, food safety and improving community health.

Effect of Substituents and Role of a Proton Donor in the Electroreductive Cleavage of N-O Bond Catalyzed by Metal Complexes

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The development of molecular catalysts for the electrochemical activation of small molecules and, more broadly, for bond activation focusses on understanding the factors that lower overpotential and enhance catalytic rate constants. Key considerations include the role of cofactors such as proton donors and, in the case of transition metal complexes, the electronic effects of ligand substituents.

This presentation will focus on N–O bond activation for the reductive deoxygenation of critical substrates like nitrous oxide (N_2O) and pyridine N-oxide. N_2O, a kinetically inert greenhouse gas, serves as a model for reductive N–O bond cleavage. Pyridine N-oxide reduction is also of interest due to its broad applications in synthesis, where selective and energy-efficient deoxygenation is needed.[1]

Previous studies have shown that rhenium bipyridine triscarbonyl complexes and iron tetraphenyl porphyrins (TPPFe) function as effective molecular electrocatalysts[2,3] or photocatalysts[4] for these reactions in the presence of a proton donor.

Focusing first on rhenium bipyridine triscarbonyl complexes, we will examine how ligand substituents influence catalytic activity in N_2O reduction, as well as the role of water as a proton donor, shedding light on the N–O bond activation mechanism.

We will then explore the impact of proton donors on deoxygenation using TPPFe as a catalyst. Our findings reveal that acids of varying strengths accelerate N–O bond cleavage, yet intriguingly, their pKa has minimal effect. This suggests that hydrogen-bond-assisted N–O bond cleavage, rather than conventional protonation, drives the reaction.[5]

Finally, we will discuss the extension of these insights to the reductive deoxygenation of pyridine N-oxides.

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New Antibody targeting human telomeric G-quadruplex DNA

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Genomic DNA has the capacity to form alternative structures to the canonical double helix. Among them G-quadruplexes (G4s) are tetrahelix structures that arise from G-rich genomic regions and result from the self-assembly of guanine residues into quartets, which are further stabilized by π-stacking interactions and coordination with metal cations such as K^+ or Na^+. Numerous *in vitro* studies have shown that G4s are highly susceptible to adopt multiple topologies, which exist in dynamic equilibrium. G-quadruplexes are known to play crucial roles in various cellular processes, including transcription regulation, DNA replication, and telomere maintenance. Dysregulation of G4 structures has been linked to several diseases, such as cancer and neurodegenerative disorders.

To investigate the structural and functional properties of G4 DNA in cells, few G4 antibodies have been identified. Most of them, including commercially available BG4, recognize the G4 structure versus duplex DNA but are not specific for a particular topology, in particular to differentiate between parallel and antiparallel G4 conformations[1]. To develop new antibodies specific to antiparallel conformation, we have used constrained antiparallel G4 telomeric biomolecular system[2] which has been found highly stable allowing the selection of antibodies using phage display method.

In this communication, we will show the use of Elisa and Bio-Layer Interferometry for the studies of the affinity of two selected antibodies and we have demonstrated that these two new antibodies are highly selective for G4 telomeric DNA versus duplex and single-stranded DNA. Furthermore, these antibodies have been used for cell imaging to detect telomeric G4 DNA.

The antibody was now marketed by Idylle under the name Anti-TeloG4 – Antibody

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Non specificity of I-motif ligands and antibody demonstrated by biophysic methods: Bio-Layer Interferometry (BLI), FRET, pull-down.

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i-Motifs of DNA (hereafter, *i*-DNA), known *in vitro* for nearly three decades, are unusual, fourstranded structures, in which cytosines are intercalated *via* a stack of hemi-protonated C–C base pairs (CH^+:C) (Fig. 1A, B). Some of these structures have been well characterized *in vitro* but their biological relevance is being investigated.

Relatively few molecules were reported to interact with i-DNA. The main issues in this regard are the strong pH-dependency, flexibility, polymorphism and complex folding behavior of i-DNA that introduce potential bias into screening methods. In particular, low-pH conditions used to induce the formation of i-DNA can increase the non-specific interactions and afford false-positive compounds. The interactions of the molecules reported as i-DNA ligands were demonstrated by FRET, pH transition or thermal melting methods but few affinity constants were measured.

In this context, we have developed a method to synthetize a constrained structure of iDNA of the human telomeric sequence (hTeloC) which was found more stable in particular at neutral pH. Using Bio-Layer Interferometry (BLI), we were able to screen and study the interactions between i-DNA and already reported ligands (TMPyP4, mitoxantrone, IMC-48, berberine, *etc*) at physiologically relevant pH. We demonstrated that none of the reported ligands were shown to discriminate between folded and unfolded *i*-motif structures [1,2]. In fact, at acidic pH, the interaction between the ligand and i-DNA were mostly governed by electrostatic interactions due to the protonation of many ligands, which can strongly increase their non-specific nucleic acid binding.

In a similar context, we also showed by using BLI that commercial *i*-motif antibody (*i-Mab*) is not able to recognize selectively the *i*-motif structure. These results were confirmed by other bi-physic technics: FRET, Circular dichroism, Pull down test [3].

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P09

Contrôle du potentiel électrique de surface d'un verre de Ge-Sb-S-Na par polarisation thermique

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Un traitement de polarisation thermique est une méthode efficace pour immobiliser des charges électriques dans une matrice vitreuse. Ces charges, fixées à la surface et au cœur du réseau vitreux, permettent d'ajouter une fonction électrique statique au matériau. Contrôler spatialement la distribution des charges, en jouant sur les paramètres du traitement et la géométrie des électrodes, rend possible la structuration des propriétés électriques de la surface du verre.

Dans le présent travail, un verre de chalcogénure de composition 99% (Ge25Sb10S65) 1%Na a été synthétisé et traité par polarisation thermique en utilisant différents voltages et géométries de l'électrode. Les modifications structurales induites dans la matrice vitreuse ont été étudiées par microscopie Raman et réflectivité infrarouge. La distribution des charges a été évaluée par une combinaison de techniques de génération de second harmonique (SHG) et de Microscopie à Sonde de Kelvin (KPFM).

Les analyses structurales ont révélé des modifications de la composition du verre dues au déplacement de cations mobiles de sodium dans les régions en contact avec l'électrode. Les analyses SHG des verres traités ont montré différentes orientations des champs électriques induits présentant des composantes planaires et longitudinales. Les potentiels électriques de surface ont été caractérisés par les mesures KPFM. L'utilisation d'électrodes microstructurées a permis un contrôle à l'échelle micrométrique du signe et de l'intensité des potentiels électriques de surface. L'ensemble de ces données nous montre que le contrôle de la position, du signe et de l'intensité des potentiels électriques de surface est possible grâce au contrôle des courants de surface qui apparaissent lors de la polarisation thermique du verre.

Modeling CO_2 Gas Hydrate using Molecular Dynamics in combination with Deep Neural Network Potentials

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Gas hydrates are of significant interest to the scientific community due to their potential hazards and their implications in energy storage and environmental applications. However, their structural complexity and size make their thearical modeling particularly challenging. Density Functional Theory (DFT) remains the most accurate method to model such systems, but its high computational cost limits its use for large-scale molecular dynamics (MD) simulations. Previous work by Nicolas Cinq et al. [1] introduced a DFTB (Density Functional Tight Binding) parametrization tailored for gas hydrates to reduce computational time, though with some compromise in accuracy compared to full DFT calculations. To overcome this limitation between accuracy and computational cost, Deep Neural Network Potentials (DNNPs) have emerged as a promising alternative, offering DFT-level accuracy with significantly reduced computational demands. In this study, we first train a deep neural network using **DeePMD-kit v2** [2] to reproduce DFT-calculated potential energy surfaces for CO_2 hydrates. Then, we perform molecular dynamics simulations using this DNNP, achieving both high accuracy and computational efficiency. Our results demonstrate that DNNPs can faithfully reproduce DFT-quality dynamics for CO_2 gas hydrates. These findings highlight the potential of DNNPs as a powerful tool for simulating complex properties of gas hydrate including phase diagram, multi-gas hydrates and water/hydrate interfaces, paving the way for efficient and accurate large-scale simulations.

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Molecular mechanism of allostery in E. Coli dihydrofolate reductase (DHFR)

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In some proteins, a perturbation at a site away from the active site can regulate the activity of the protein. The communication between the two distant sites is called allostery. This regulation typically occurs through ligand binding, but the effect of a distal mutation on the activity of a protein can be seen as latent allostery. Since 1964, several models have been proposed to describe allostery, but its explanation at the molecular level is still unknown. In this study, we focus on E. coli dihydrofolate reductase (DHFR), in which Benkovic showed that distal mutations at G121 site, more than 1 nm away from the active site, affect the rate of hydride transfer between the NADPH cofactor and the protonated H3F+ folate, which is the second part of the chemical step in the enzyme's catalytic cycle [1]. We use replica-exchange molecular dynamics simulations to show that the effect of G121V on hydride transfer can be explained by a conformational equilibrium shift due to steric interactions, from conformations in which the NADPH and H3F+ cycles are parallel to conformations in which they are perpendicular. Using Oanca et al.'s implementation of EVB for Gromacs [2], we then demonstrate that parallel conformations are much more reactive than perpendicular ones and that the equilibrium shift is consistent with a MWC-type model of allostery [3]. Using out-of-equilibrium MD simulations, we finally propose a molecular mechanism for the transition pathway from the parallel conformation of WT to the perpendicular conformation of G121V and provide a kinetic model for this mechanism. To our knowledge, this is the first molecular mechanism of allostery in EcDHFR and one of the first molecular mechanisms of allostery in any system.

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P12

Unveiling the Role of Hydride Bridges in the Electrical and Nonlinear Optical Behavior of Hydride Nanoclusters: A Theoretical Perspective

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In this study, we explore the geometric structures, electronic properties, and both static and dynamic nonlinear optical (NLO) characteristics of a novel series of eight nanocluster copper hydrides, $Cu_3L_xL'_yH_n$. The first hyperpolarizabilities, linked to Hyper-Rayleigh Scattering (HRS), Second Harmonic Generation (SHG), and the Electro-optic Pockels Effect (EOPE), were systematically investigated, along with second hyperpolarizabilities related to ElectricField-Induced Second Harmonic Generation (EFISHG), Degenerate Four-Wave Mixing (DFWM), and DC-Kerr effects. These NLO properties were calculated using density functional theory (DFT), providing detailed insights into the advanced optical behavior of these nanoclusters. For the first time, we demonstrate that the presence of hydride bridges plays a pivotal role in enhancing the stability of copper nanoclusters while also significantly boosting their nonlinear optical responses. Furthermore, we identify a promising potential application of copper hydride nanoclusters in photonics, further extending their relevance to modern material and optical sciences.

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P13

A photosynthetic fuel cell used as a bio-electric power supply in an electrodialysis process

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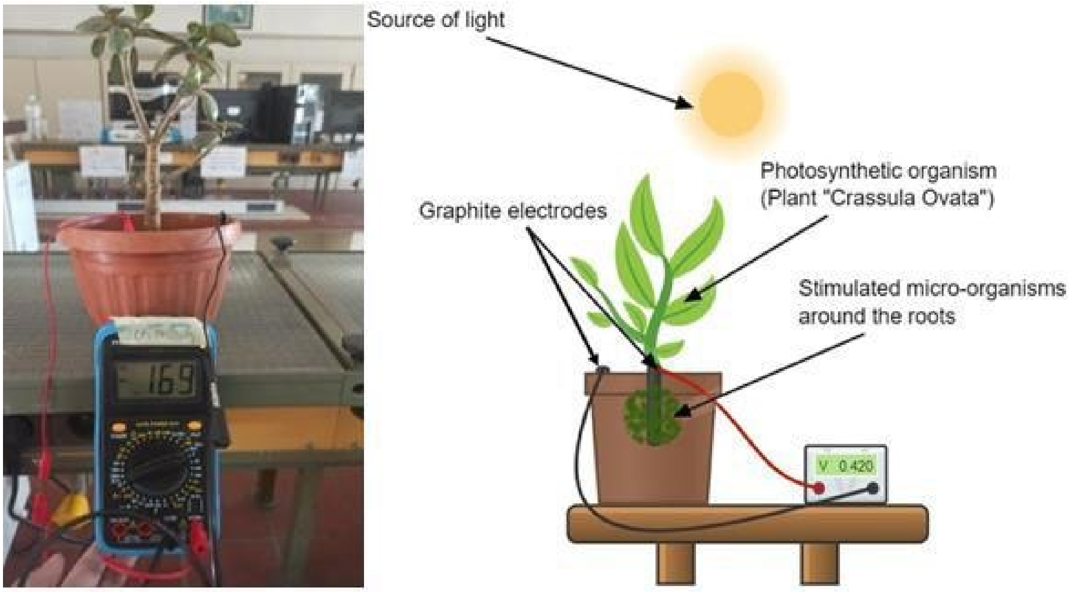
The bio-photovoltaics is an advanced green alternative energy that draws the attention to many electrochemical researchers nowadays, considering its innovative nature and potential different applications. In this context, a photosynthetic fuel cell has been elaborated and conceived for the production of bio-electricity by using the natural photosynthetic process. This bioelectrochemical device consists of a carbon-based bioanode and biocathode which are dipped inside a pot filled with garden soil, in which *Crassula Ovata* is planted. The bioanode is placed close to the roots of the plant, whereas the biocathode is placed at the edge of the pot. The production of the bio-electricity is achieved at the bioanode by the oxidation of the organic matter (glucose resulting from the photosynthesis) by means of the microorganisms present in the soil. The plant acts as a stimulant for the microorganisms via photosynthesis, while the photosynthetic oxygen is reduced at the biocathode. The performance of this bioelectric power supply has been observed in different lighting conditions and also in absence of the plant. The results obtained so far, show that the photosynthesis is an effective stimulant for the performance of this bio-electric device. However, this bio-electrochemical process struggles from the electron transport due to the lack in performance at the bioanode. Hence, an appropriate amplification system is employed to improve the low bio-electricity generated during the photosynthesis. The performance of this bio-electrochemical device has been tested successfully in an electrodialysis process.



(a) **(b)**

Figure: Photosynthetic fuel cell; (a) Experimental set up with the plant"Crassula Ovata", (b) Representative diagram of its components

P14

When water molecules play with ions : a field gradient NMR approach to investigate Water-in-Salt-Electrolytes dynamics

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Dissolving a salt into water leads to electrolytes which possess much more complex behaviors than the simple sum of their counterparts, leading to fascinating and unexpected properties. This is the consequence of *i*) the limit of solubility (from traces up to few water molecules per salt pair) and *ii*) the relative specific interactions of water molecules, cation and anions (such as ions inducing ordering or disordering of water molecules in their solvatation sheath...). To this respect, studying cesium halide salts dissolved in water up to their respective limit of solubility allows to cover specific electrolyte features : very concentrated electrolytes, chaotropic to kosmotropic ions ... NMR is then a powerful tool for such studies, (1) allowing to get individual informations on each species (averaged charge distribution, interaction, reorientational dynamics) and also the individual self-diffusion coefficients which are generally measured by pulsed field gradient NMR (PFG-NMR)(2) which is a very powerful method to measure nuclei such as H, F or Cs (see figure). However, to measure self-diffusion coefficients of ions like Cl^-, Br^- or I^-, this method is not suitable (these nuclei are strong quadripolar and their relaxtion times are too short), and we developped the strayfield (STRAFI) NMR method which exploits the natural gradient inside a cryogenic magnet.

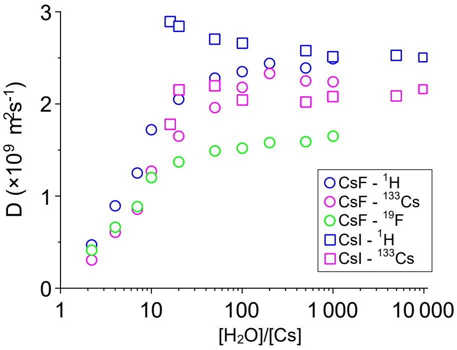

Figure : self-diffusion coefficients of water and ions in CsF *and CsI as measured by PFG NMR (300K).*

Then the translational mobility of each species inside electrolytes can be measured to dvelve individual dynamic abilities, and the complementary measurements of viscosity and ionic conductivity allows to reach fundamental data such as hydrodynamic radius, dissociation ratio, selectivity of ionic transport …

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Modelling Ni(II) sorption onto Cox clay rock under EDTA perturbation.

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The Cigéo project, a 500 meters deep underground disposal, is considered in France for management of radioactive waste [1]. The confinement of radionuclides (RNs) is ensured by several barriers, including Callovo-Oxfordien clay rock as the ultimate geological barrier. RNs mobility is quantified through laboratory and *in situ* experiments. Then modelling in near-field and far-field of disposal is performed, based on geochemical conditions and perturbation effects (hydraulic, thermal, chemical). The present work focuses on the effect of a strong complexing agent, EDTA, considered as co-contaminant. Its effect is well described on various compounds: Eu, Th, U [2]. Yet, the effect of EDTA on the retention of ^{59}Ni, a potential dose contributor, exhibits specific mechanisms. We will present recent development on modelling of such geochemical system under perturbation.

Retention of cations is described by sorption isotherms as a function of pH or concentrations (Fig. 1). These isotherms are commonly modeled using the 2 SP-SCM-NE model [3]. The case of Nickel display two specificities. First the retention is due to several mechanisms, including fast reversible adsorption on surfaces, and slow "non"-reversible incorporation in mineral phases [4]. Secondly, the retention is closely affected by other divalent present in the geochemical media (Co, Fe, Mn…) which are difficult to model simultaneously. The retention of Ni at low EDTA concentration is one order of magnitude higher than expected without consideration of Zn (plateau on Fig. 1). At high EDTA concentration ($>10^{-3}$ M) the modeled isotherm fits the experimental one when considering an EDTA sorption [5]. At intermediate EDTA concentration, Ni retention decrease because of complexation of free Ni^{2+} in solution. Still, the model disagrees with experimental data because of the very high complexation constant of log $\beta\{[Ni\text{-}EDTA]^{2-}\}$, compared to other [M-EDTA] complexes. Hence, the sorption model seems hampered by the sole thermochemical considerations. Several phenomena may be considered to account for such disagreements between data and model. First, the presence of divalent buffers naturally present in the geochemical media (Zn, Mn, Fe) is poorly documented. Secondly, the over-estimation of the Ni availability in the natural media is difficult to predict accurately in the perturbed system.

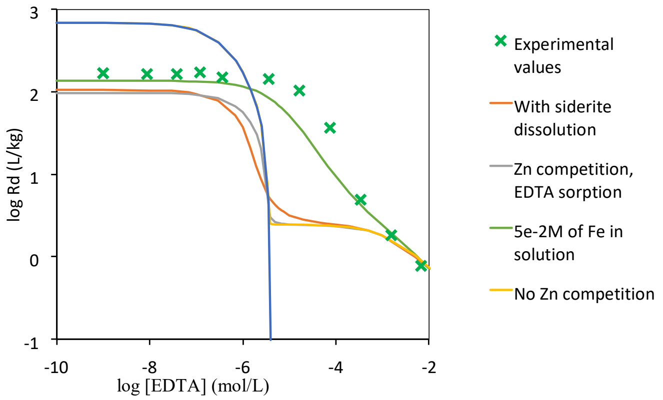

Figure: Retention isotherm of Ni on Cox clay rock as a function of EDTA concentration. Effect of hypothesis on the predictive modelling of the geochemical system under perturbation.

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Exploring the Impact of Molecular Configuration on Optoelectronic Properties in Ph-subPC/C60 Organic Solar Cells

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Organic solar cells represent a very promising technology for low-cost, flexible, and lightweight solar energy harvesting. The morphology of the donor-acceptor interface is at the heart of the performance of OSCs and is fundamentally responsible for the efficiency of charge separation and transport therein. This interface morphology and electronic structure presents a big experimental challenge toward its precise characterization and understanding.

In this regard, the design of new materials that can further optimize these interfaces is very important. This contribution deals with phenoxysubphtalocyanine-Ph-subPC, a derivative of the wellknown boron subphthalocyanine chloride, subPC. The core-expanded six-membered ring in the design of Ph-subPC may further improve its electronic property compared to its forerunner. Here, we combined the newest frontier orbital energy-level molecular design for a Ph-subPC with the C60 fullerene and investigated how these new molecular arrangements at the donor-acceptor interface in OSCs affect optoelectronic properties.

In this work, we model different configurations of the Ph-subPC/C60 interface using DFT and time-dependent DFT. We name those configurations B and U, in which B represents the C60 positioned on the convex surface of Ph-subPC and U represents C60 embedded in the concave surface. We observe from simulations that changing the orientation of C60 with respect to Ph-subPC significantly influences important photovoltaic properties like absorption spectrum, open-circuit voltage, and exciton binding energy.

The current study also investigated the effect of molecular arrangement and orientation on the photoelectric performance properties, including binding energy, frontier molecular orbital energies, UVVis absorption spectrum, and exciton binding energy. In comparison with the subPC/C60 system, it has led to deeper insights into how variations in the molecular configuration could impact the electronic and optical performance of OSCs.

Key words: boron subphthalocyanine chloride, DFT, TDDFT.

P17

Study on GLDA–Metals

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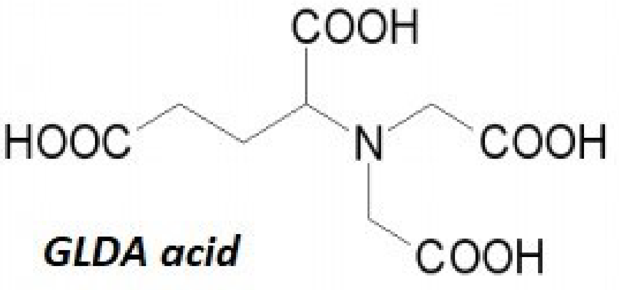
N,N-Dicarboxymethyl glutamic acid (GLDA) is an important chelating agents. Non- covalent interactions between GLDA complexed with alkali metals Li+, Na+, K+ and Rb+, were investigated with density functional theory using PBE-D3 functional. Conformational possibilities of GLDA were explored with a varying number of carboxylic pendant arms of
GLDA in close proximity to the ions. It is found that the case in which four arms of GLDA are interacting with ions is more stable than other conformations.
The objective of this study was to explore the electronic structure properties upon complexation of alkali metals Li+ Na+, K+ and Rb+ with a GLDA chelator. Interaction energies and relaxation energies, show that the stability of GLDA, complexed with alkali metals decreases down the group of the periodic table. Implicit water solvation affects the complexation of GLDA—ions leading to decreases in the stability of the complexes.



Ab initio Polaritonic Chemistry beyond qubit-platforms

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Simulating ab initio polaritonic chemistry on quantum computers presents a significant challenge due to the need for efficient encoding of strongly correlated hybrid electron-photon states within quantum circuits. In this work, we introduce compact, physically motivated quantum circuit ansätze tailored to different quantum architectures and integrate them with the State-Averaged Variational Quantum Eigensolver (SA-VQE) to compute multiple polaritonic eigenstates. We develop and benchmark three circuit architectures designed for distinct quantum hardware platforms: (i) a qubit-based formulation compatible with standard gate-based quantum hardware, (ii) a quditbased approach leveraging higher-dimensional quantum states, and (iii) a hybrid qubit-qumode scheme utilizing continuous-variable quantum systems. To validate our methodology, we compute the four lowest-lying eigenstates of a cavity-embedded H_2 molecule, successfully capturing essential polaritonic effects, including light-induced avoided crossings and conical intersections.

Exchange-Correlation Functional as the Hidden Variable in Borosilicate Glasses Neural Network Potentials

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Borosilicate glass is a model system for various multicomponent oxide glasses with wide industrial and technological applications, ranging from cookware, labware, to optical lenses, bioactive coating, and nuclear disposal, owing to their low thermal expansion coefficient and high chemical resistance. However, their atomic-scale structure is difficult to resolve, primarily because of complexity of boron coordination chemistry [1]. In particular, the distribution between the trigonal [BO_3] and tetrahedral [BO_4] is highly sensitive to both composition and the underlying description of atomic interactions. Neural network potentials (NNPs) have emerged as a promising approach to overcome the trade-off effect between accuracy and computational cost, offering ab initio molecular dynamics (AIMD) level accuracy with scalability of classical molecular dynamics (CMD). However, their reliability depends critically on the quality of the density functional theory (DFT) reference datasets used for training. We investigate the influence of exchange-correlation (XC) functional in DFT on the ability of NNPs to reproduce boron coordination in borosilicate glasses. Reference datasets were generated using DFT single-point calculations using a range of functionals including PBE, PBEsol, r^2SCAN, PBE0 and MN15. Separate NNPs were trained on each dataset. We systematically compared their performance in the prediction of structural properties, densities and boron coordination number. Our results demonstrate that different XC functionals yield markedly different boron coordination statistics. Notably, PBEsol outperformed other functionals, including more advanced ones, in predicting four-fold boron coordination. However, an average relative error of around 20% from NNP trained on PBEsol with respect to experimental data [2] remains across all compositions. Therefore, these findings highlight that the choice of XC functional is a decisive step in constructing transferable machine learning potentials, while also exposing the limitations of current DFT approaches in capturing boron coordination chemistry in borosilicate glasses.

References (5 maximum)

[1] Wang, M. et al. **Journal of Non-Crystalline Solids** 498, 294–304 (2018).
[2] Smedskjaer, M. M. et al. **J. Phys. Chem. B** 115, 12930–12946 (2011).

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