RTG 2721

^{1,2,3}H: Interdisciplinary Perspectives on Hydrogen Isotopes

Book of Abstracts

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Programme

^{1,2,3}H: Interdisciplinary Perspectives on Hydrogen Isotopes

23 – 25 March 2026, Leipzig, Germany

Monday 23 March (timings are CET)

08:00–08:45	Registration
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09:45–10:15	Tanja Gulder **Electrochemical Hydrogen–Deuterium Exchange: Towards Sustainable Approaches for Late-Stage Isotope Labeling**
10:15–10:30	Junsu Ha **High-temperature hydrogen isotope separation enabled by locally flexible gates in tightly confined microporous metal-organic frameworks**
10:30–11:00	Coffee Break
11:00–11:30	Hyunchul Oh **Advanced MOF Strategies for Hydrogen Isotope Separation**
11:30–11:45	Sibo Chetry **Structural Determinants of Dihydrogen Adsorption and Isotopologues Separation in Metal-Organic Frameworks**
11:45–12:00	Hrittik Karmakar **Infrared Photodissociation Spectroscopy of $Cu_2(OAc)_2(D_2)_n^+$ and its Isotopologues**
12:00–12:30	Michael Hirscher **Adsorption-Based Separation of Gaseous Hydrogen Isotopologue Mixtures Investigated by Thermal Desorption Spectroscopy**
12:30–13:30	Lunch
13:30–14:00	Daniel Obenchain **Ligand Exchange in Gas-Phase Molecular Hydrogen Complexes Influenced by Isotopic and Spin-Isomer Effects**
14:00–14:15	Dennis El Mouzawak **Ion Soft-Landing of Undercoordinated Metal Complexes: Spatial Profiling, Ion Beam Control, and Stabilization**
14:15–14:30	Maria Chiara Crimella **Deposition of Charged Microdroplets to Quantify Charge Separation of Salts in the ESI Process**
14:30–15:00	Martin Beyer **Hydrogen-Deuterium Exchange in Charged Water Clusters**
15:00–15:30	Coffee Break
15:30–16:00	Linda Zhang **Distinct Lattice Responses and Adsorption Dynamics of Hydrogen Isotopologues in a Flexible Triazolate MOF**
16:00–16:15	Pranjit Das **Hydrogen Isotope Adsorption in V-Doped MIL-53(Al) Using *In Situ* EPR Spectroscopy**
16:15–16:30	Akira Taguchi **H_2-D_2 Separation in 8-membered Ring Zeolites (CHA, RHO, and LTA (4A)) at Mild Temperatures**
16:30–17:00	Irena Senkovska **Particle Size Tuning of Responsive MOFs as a Tool to Achieve Efficient Gas Separation Performance**
17:30–19:30	**Poster Session**

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09:45–10:15	Inez Weidinger **The Role of Protons in Electrocatalysis**
10:15–10:30	Kwangjin An **Catalyst Design for Liquid Organic Hydrogen Carriers (LOHCs)**
10:30–11:00	Coffee Break
11:00–11:30	Cornelius Fischer **Hydrogen Isotope (^{1}H, ^{2}H, ^{3}H) Interactions with Microporous Materials: Experimental and Analytical Insights**
11:30–11:45	Alexander Feige **Electron Diffraction as an Alternative to Neutron Methods for Hydrogen Isotope Identification**
11:45–12:00	David Egloff **From Experience to Engineering: The Evolution of Safe and Refined Tritium Handling**
12:00–12:30	Genrich Zeller **Raman Spectroscopy and Microscopy of Tritiated Samples**
12:30–13:30	Lunch
13:30–14:00	Olga García Mancheño **Late-Stage Photocatalytic Hydrogen Isotope Exchange and H-Isotope Effects Towards Selective Reduction Reactions**
14:00–14:15	Hannah Buttkus **Hydrogen Isotope Effects Used to Reveal Vibrational Signatures of a Microsolvated Hexafluorophosphate Anion**
14:15–14:30	Erik Butenschön **What ^{1}H & ^{2}H NMR Reveals About Enzymatic PET-Degradation**
14:30–15:00	Detlev Belder **Integrated Chemical Microlaboratories: A Key Technology for Automated, Safe, and Sustainable Reaction Processing**
15:00–15:30	Coffee Break
15:30–16:00	Jörg Meyer **New Insights into the Volume Isotope Effect of Ice Ih from Polarizable Many-Body Potentials**
16:00–16:15	Muhammad Fernadi Lukman **Local Structure Insight of Flexible Cu^{2+} doped ZIF-8 and Its Application to Hydrogen Isotopologues Detection**
16:15–16:30	Nils Hertl **Mode Selectivity in Electron Promoted Vibrational Relaxation of Chemisorbed Hydrogen on Molybdenum and Tungsten Surfaces**
16:30–17:00	Alexandra Becker **Preparation and Characterization of Solid Low-Activity Tritium-Loaded Samples**
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Wednesday 25 March (timings are CET)

09:00–09:45	Melanie Schnell **H-Isotope Dependent Effects Revealed with High-Resolution Molecular Spectroscopy**
09:45–10:15	Anne B. McCoy **Deciphering Spectral Signatures of Proton Delocalization in Hydrogen-Bonded Complexes**
10:15–10:30	Milena Barp **Vibrational Signature of Shared Hydron in Deprotonated HFIP Dimer and Trimer**
10:30–11:00	Coffee Break
11:00–11:30	Grégory Schneider **Graphene and its Interactions with Protons and Hydrons**
11:30–11:45	Maria Judith Caisachana Lozada **Effects of Mechanical Strain and Local Curvature on Hydrogen Isotope Selectivity in Graphene Membranes**
11:45–12:00	Dario Calvani **Enhanced and Selective Unidirectional Proton Transport via Covalent Benzenesulfonic Functionalized Nanoporous and Pristine Graphene**
12:00–12:30	Thomas Kühne **Quantum Mechanics in a Glass of Water**
12:30–13:30	Lunch
13:30–14:00	Thomas Heine **Thermodynamic Limits of Chemical Affinity Sieving**
14:00–14:15	Felix Moncada **Nuclear Orbitals within the Born-Oppenheimer Approximation**
14:15–14:30	Daniela Mondonico **Design Principles for Isotopologue-Selective Membranes in Aqueous Environment: The Interplay Between Pore Size and Functional Group Chemistry**
14:30–15:00	Hoi Ri Moon **Metal–Organic Frameworks as Quantum Sieving Platforms for Next-Generation Hydrogen Isotope Separation**
15:00–15:30	Closing
15:30–17:30	**Lab tour**

Talks

Day 1 — 23 March 2026

Mon 09:00–09:45: Keynote Talk – Stefan Kaskel

Porous Materials for Isotope Separation

Stefan Kaskel

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Porous materials are used in industry for various gas and liquid phase separations. While zeolites and activated carbons are established adsorbents for industrial applications, in recent decades a plethora of novel tailorable materials was developed such as Metal-Organic Frameworks (MOFs), acknowledged by the Nobel Prize in 2025, ZIFs, COFs, PAFs, and many more.

An emerging application of porous materials is the separation of isotopologues. In particular H_2/D_2 and H_2O/D_2O separations received considerable attention in recent years. Despite the use of D_2 is mostly driven by niche applications in biomedicine and electronics, recent efforts in nuclear fusion reactor technology foster intensified efforts targeting tritium production and $^6Li/^7Li$ separation.

A fascinating feature of selected MOFs is their ability to open the pores only for selected molecules as a response to guest inclusion leading to an almost ideal separation selectivity.[1] In that respect, recently various MOFs were discovered demonstrating selective pore opening for D_2 vs. H_2 or kinetic separation principles based on different adsorption rates.

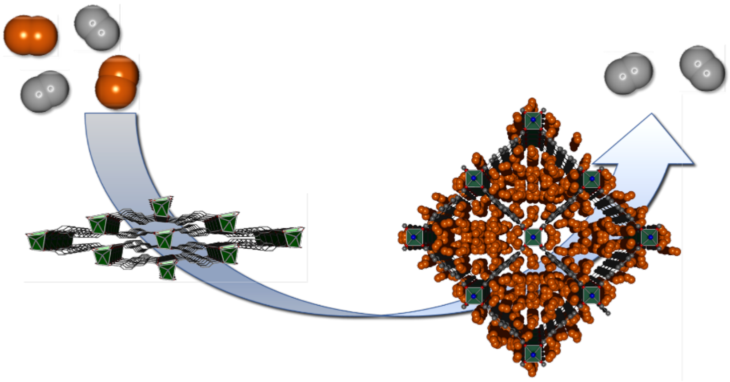

Figure 1: Flexible MOFs such as DUT-8 open their pores selectively for D_2 leading to a high D_2/H_2 adsorption selectivity.[2,3]

The presentation provides an overview on various porous materials and their application to isotope separation.

[1] I. Senkovska, V. Bon, A. Mosberger, Y. Wang, S. Kaskel, *Adv. Mater.* **2025**, 37, 2414724.

[2] L. Bondorf, J. L. Fiorio, V. Bon, L. Zhang, M. Maliuta, S. Ehrling, I. Senkovska, J. D. Evans, S. Kaskel, T. Heine, M. Hirscher, *Sci. Adv.* **2022**, 8 (15), e-abn7035.

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Mon 09:45–10:15: Invited Talk – Tanja Gulder

Electrochemical Hydrogen–Deuterium Exchange: Towards Sustainable Approaches for Late-Stage Isotope Labeling

Tanja Gulder

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The incorporation of deuterium atoms into organic molecules has emerged as a transformative strategy in modern synthetic chemistry, driven by its broad utility in physical organic studies, medicinal chemistry, and chemical biology.[1] Traditional approaches to deuterium incorporation often rely on multi-step syntheses using pre-functionalized substrates, which suffer from poor atom economy and limited tolerance to functional groups.[2] Hydrogen isotope exchange (HIE) offers a promising alternative for late-stage functionalization.[3] Current protocols for HIE, however, typically require harsh conditions, strong acids or bases, and transition-metal catalysts, which restrict their applicability. Recent advances in photocatalytic and electrochemical HIE have enhanced sustainability and operational simplicity, aligning with the principles of green chemistry.

This talk will highlight our group's recent advances in developing hydrogen-deuterium exchange reactions utilizing electrochemistry.[4] Our strategies help push the boundaries of chemical space, granting access to a rich diversity of novel chemical structures that often cannot be approached by our current standard method repertoire.

[1] a) J. Atzrodt, V. Derdau, T. Fey, J. Zimmermann, *Angew. Chem. Int. Ed.* **2007**, *46*, 7744-7765; b) S. Kopf, F. Bourriquen, W. Li, H. Neumann, K. Junge, M. Beller, *Chem. Rev.* **2022**, *122*, 6634-6718.

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[3] G. Prakash, N. Paul, G. A. Oliver, D. B. Werz, D. Maiti, *Chem. Soc. Rev.* **2022**, *51*, 3123-3163.

[4] a) Y. Ni, J. Lebelt, M. Barp, F. Kreuter, J. Jin, H. Buttkus, M. Kretzschmar, R. Tonner-Zech, K. R. Asmis, T. Gulder, *Angew. Chem. Int. Ed.* **2025**, e202417889; b) J. Lebelt, T. Gulder, German Patent Application, DE102025123173.7, Germany, **2025**.

Mon 10:15–10:30: Contributed Talk – Junsu Ha

High-temperature hydrogen isotope separation enabled by locally flexible gates in tightly confined microporous metal-organic frameworks

Junsu Ha,[a,b] Minji Jung,[c] Jaewoo Park,[c] Shinyoung Kang,[d] Mingyu Jeon,[d] Jihyun Park,[c] Jihan Kim,[d] Hyunchul Oh[,*,c] Hoi Ri Moon[*,b]

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[c]*Department of Chemistry, Ulsan National Institute of Science and Technology (UNIST), Ulsan 44919, Republic of Korea.*
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Conventional kinetic quantum sieving method based on rigid frameworks exhibit high performance only at cryogenic temperatures near the liquefaction temperature (20 K) of hydrogen isotopes, due to their weak binding energies on the outer surface of porous materials. In this study, our strategy to achieve high operation temperatures, as well as large uptake toward deuterium, involves the introduction of diffusion barrier to the apertures of MOFs containing large cavities. We prepared a series of isoreticular MOFs (Cn-IRMOF, n = 4 and 5), featuring butoxy and pentoxy functionalized terephthalate as the locally flexible kinetic barriers to achieve higher separation temperatures. Their kinetic behavior was analyzed using hydrogen sorption measurements and thermal desorption spectroscopy. Among the series of Cn-IRMOF, C5-IRMOF, which has crystallographically disordered pentoxy gates, exhibits different pore limiting envelope from 1.5 to 3.6 Å depending on temperature, which was proved by molecular dynamics simulation. This provides the most effective confinement phenomenon for KQS at a significantly higher temperature of 100 K, with meaningful D2/H2 selectivity and a D2 uptake of approximately 1.0 mmol/g.

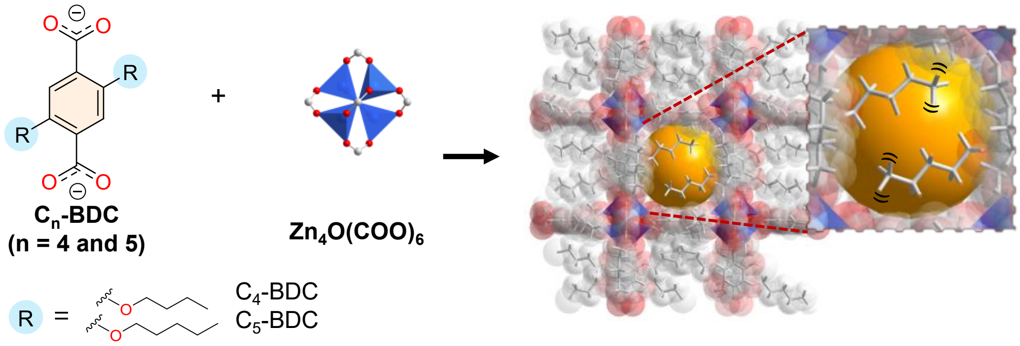

Figure 1: Schematic images of Cn-IRMOF structure consisting of Zn4O cluster and Cn-BDC with flexible alkyl chains.

Mon 11:00–11:30: Invited Talk – Hyunchul Oh

Advanced MOF Strategies for Hydrogen Isotope Separation

Hyunchul Oh

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Efficient separation of hydrogen isotopes is crucial for fusion energy, neutron science, and the electronics industry, but conventional cryogenic distillation is extremely energy-intensive. Metal–organic frameworks (MOFs) provide a tunable platform for engineering quantum effects, adsorption energetics, and mass transport from the atomic to the particle scale. In this presentation, I will introduce a set of "isotope-responsive" MOF design strategies, organized into two regimes: enhanced separation at cryogenic temperatures and improved performance at relatively higher temperatures.

In the cryogenic regime, three complementary approaches are highlighted. First, adsorption-induced site transformation in microporous MOFs is elucidated by combining isotherms with neutron powder diffraction, revealing a sequence of adsorption sites that boost D_2/H_2 selectivity at low temperature (*JACS*).[1] Second, isotope-selective condensation in mesopores may exploit the delayed capillary condensation of H_2 relative to D_2, leading to large D_2 uptakes and high selectivity.[2] Third, particle-size control in Ni-MOF-74 is used to tune the diffusion path length and contact time; by shrinking crystal size, diffusion profiles change, and isotope selectivity is enhanced under short exposure and low-temperature conditions.[3]

In the higher-temperature regime, two lattice-level design concepts are emphasized. A lattice-driven gating effect in thermally expandable frameworks such as Cu(II) ZIF-*gis* harnesses thermal lattice expansion to switch between closed and open pore states (gate opening), enabling kinetic quantum sieving near LNG liquefaction temperatures and above (*Nat. Comm.*).[4] In parallel, an isomerism-based ligand exchange strategy preserves the Ni_2O_2 framework topology while substituting positional isomers of the dobdc linker, subtly modifying the adsorption potential landscape and delivering improved D_2/H_2 separation performance at and above 77 K. [5]

Together, these cryogenic and elevated-temperature strategies define a coherent toolbox for designing next-generation MOF adsorbents tailored to specific process windows and performance targets in hydrogen isotope separation.

[1] Jin Yeong Kim … Hyunchul Oh*, *JACS* **2020**, *142*, 13278.
[2] Jaewoo Park … Hyunchul Oh*, *Manuscript in preparation.* **2026**
[3] Hyerin Lee … Hyunchul Oh*, *Manuscript in preparation.* **2026**
[4] Minji Jung … Hyunchul Oh*, *Nat. Comm.* **2025**, *16*, 2032.
[5] Sungyeop Jung … Hyunchul Oh*, *Manuscript in preparation.* **2026**

Mon 11:30–11:45: Contributed Talk – Sibo Chetry

Structural Determinants of Dihydrogen Adsorption and Isotopologues Separation in Metal-Organic Frameworks

Sibo Chetry[a],*, Prantik Sarkar[b], Michael Hirscher[b], Harald Krautscheid[a]

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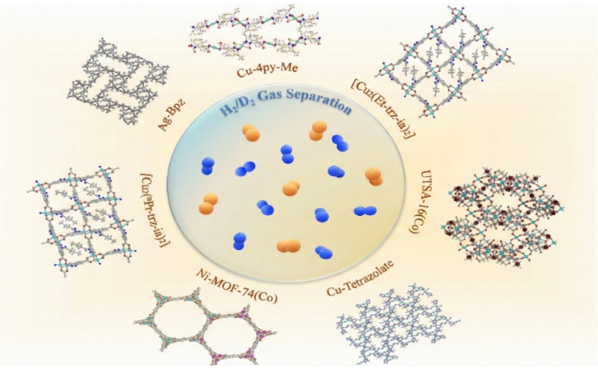
The purification of deuterium (D_2) is essential for nuclear technology and medicinal chemistry, yet conventional cryogenic distillation remains energy-intensive with low selectivity ($S \approx 1.4$) [1]. This study systematically investigates how structural features in metal-organic frameworks (MOFs) specifically ultra-micropores, open metal sites (OMS), and framework flexibility influence D_2/H_2 separation efficiency [2]. We employed Thermal Desorption Spectroscopy (TDS) to evaluate various MOF geometries under cryogenic conditions. Our findings demonstrate that ultra-microporous frameworks facilitate D_2 preference through kinetic quantum sieving (KQS), leveraging the smaller effective radius of heavier Isotopologues in confined spaces [2]. Notably, Ni-MOF-74(Co) exhibited exceptional performance, achieving a selectivity of S = 52 at 77 K [2]. This high efficiency is attributed to chemical affinity quantum sieving (CAQS) at the open metal sites, where differences in zero-point energies enhance the adsorption enthalpy for D_2 [2]. Furthermore, we examined flexible MOFs, $[Cu_2(^{n}Pr\text{-trz-ia})_2]$ and $[Cu_2(Et\text{-trz-ia})_2]$, which displayed temperature-responsive structural transitions [2]. These materials achieved D_2/H_2 selectivity ranging from 1.4 to 2.3 at 77 K, indicating that cryogenic flexibility can be tuned for isotope discrimination [2].

In conclusion, this research establishes that the rational design of pore apertures and the integration of specific adsorption sites are vital for advancing Isotopologues separation [1-2]. By moving beyond traditional distillation, these MOF-based strategies offer a path toward more sustainable and efficient deuterium enrichment at practical operating temperatures.



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[2] Chetry, S., Sarkar, P., Bakhtian, M., Hirscher, M., & Krautscheid, H. (**2025**). Influence of Structural Determinants of Dihydrogen Adsorption and Isotopologue Separation in Metal-Organic Frameworks. *ChemRxiv*. https://doi.org/10.26434/chemrxiv-2025-8389n-v2.

Mon 11:45–12:00: Contributed Talk – Hrittik Karmakar

Infrared Photodissociation Spectroscopy of $Cu_2(OAc)_2(D_2)_n^+$ and its Isotopologues

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Dihydrogen complexation by metal cations has been extensively investigated in the context of H_2 activation.[1] More recently, dihydrogen adsorption at metal sites particularly Cu(I) within metal organic framework materials has gained attention for potential applications in H_2/D_2 separation.[2] To better understand the binding interaction that govern such isotope separation, we investigate the interaction of H_2 and D_2 with a Cu(I) paddlewheel motif under isolated gas-phase conditions, free from the influences of condensed phase environments.

In this study, we report the infrared photodissociation (IRPD) spectra of mass-selected $Cu_2(OAc)_2(H_2)_n^+$ and $Cu_2(OAc)_2(D_2)_n^+$ complexes (n = 1–2), recorded in a cryogenic ion trap at 10 K and 12 K, respectively. These measurements are complemented by harmonic vibrational analysis at the def2-TZVPP level of theory, enabling structural assignments and interpretation of vibrational features. The spectra show distinct vibrational signatures of dihydrogen isotopes, including fundamental H–H and D–D stretching bands as well as combination modes involving $Cu^+–(H_2/D_2)$. Frequency shifts and intensity patterns reveal isotope dependent effects, which are discussed in comparison to previously studied systems such as $Cu(H_2)_4^+$ and $Cu(H_2O)(H_2)_2^+$.[3,4] The results highlight the role of the acetate-based paddlewheel scaffold in tuning the strength and dynamics of H_2/D_2 binding at Cu(I) centres under isolated gas-phase conditions. These findings will be helpful to understand the role of Cu(I) sites for the separation of hydrogen isotope

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[3] J. Jin, T. Wulf, M. Jorewitz, T. Heine, K. R. Asmis, *Phys. Chem. Chem. Phys.*, **2023**, 25, 5262.

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Acknowledgements: This work was funded by the Deutsche Forschungsgemeinschaft (DFG) Project ID 443871192 – GRK 2721: “Hydrogen Isotopes, $^{1,2,3}H$”.

Mon 12:00–12:30: Invited Talk – Michael Hirscher

Adsorption-Based Separation of Gaseous Hydrogen Isotopologue Mixtures Investigated by Thermal Desorption Spectroscopy

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Separating gaseous hydrogen isotopes is one of most difficult challenges in separation technology. Porous materials with well-defined pore structure, size and apertures, as zeolites and metal-organic frameworks, can be applied for isotope separation by isotopologue selective adsorption from gaseous mixtures. Different separation principles can be utilized based on kinetic quantum sieving (KQS), chemical affinity quantum sieving (CAQS), or framework flexibility, either locally at pore aperture or structural breathing. Quantum effects are typically more pronounced at low temperatures and often temperatures below the boiling point of liquid nitrogen are required. Separation of gaseous mixtures by porous media is usually measured by breakthrough experiments, however, these require typically gram-scale samples and are extremely difficult to perform at temperatures below 77 K. Novel framework materials are often only available in milligram quantities and more sensitive techniques are required. Low-temperature thermal desorption spectroscopy (TDS), first developed in Stuttgart (Figure 1),[1] offers a high, isotope-specific sensitivity, which allows a direct measurement of the selectivity after selective adsorption from gaseous isotopologue mixtures.

The presentation will describe the setup and operation of thermal desorption spectroscopy at low temperatures after exposure to hydrogen isotope mixtures. Examples of characteristic MOFs and zeolites will demonstrate the huge versality of TDS experiments.

Figure 1: First low-temperature thermal desorption spectroscopy (TDS) experimental set-up with liquid He cooling at Max Planck Institute in Stuttgart.

[1] B. Panella, M. Hirscher, B. Ludescher, *Microporous and Mesoporous Materials* **2007**, 103, *230–234*.

Mon 13:30–14:00: Invited Talk – Daniel Obenchain

Ligand exchange in gas-phase molecular hydrogen complexes influenced by isotopic and spin-isomer effects

Daniel Obenchain, Beppo Hartwig, Jannes Niels Hasselhorn, Radek Tovtik, Nadja A. Simeth

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The smallest possible molecule that involves hydrogen atoms forming a van der Waals complex is dihydrogen itself. Complexes of dihydrogen with any binding partner are complicated by the fact that H_2 can exist in two different nuclear spin isomeric forms, one of which must retain its rotation in the complex (*ortho*-H_2, $I = 1$) whereas the other does not (*para*-H_2, $I = 0$). This results in different physical behavior and can even impact their reactivity in the gas phase [1]. Hence, seemingly simple complexes are not necessarily easy to understand. Different gas-phase spectroscopic methods have shown that *ortho*-H_2 complexes are more stable than *para*-H_2.[2,3] Even in forming van der Waals complexes, the hydrogen rotational states are preserved, and *ortho*-H_2 continues to rotate in the bound state.

In our studies involving several different H_2 complexes with aromatic van der Waals binding partners, we noticed inconsistent intensities between *para*-H_2 and *ortho*-H_2 complexes, were a ratio of 3:1 is expected. This led to a study of the formation dependence of the complexes relative to the concentration of hydrogen used in our pulsed-jet experiment. The results are consistent with previous studies of H_2 complexes, that the rotating bound state of H_2 or D_2 binds more strongly than the non-rotating state. Ligand exchange effects in the expansion can push the ortho/para ratio well beyond the normal 3:1 ratio. The same effect is found in ligand exchange experiments in D_2 complexes. These results are further complicated by the apparent difference of binding distance of the complexes, with a difference between *ortho*-H_2/*para*-H_2 and the aromatic ring ($\Delta_{r,complex}$) of about 0.2-0.3 Å.

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Mon 14:00–14:15: Contributed Talk – Dennis El Mouzawak

Ion Soft-Landing of Undercoordinated Metal Complexes: Spatial Profiling, Ion Beam Control, and Stabilization

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Ion soft-landing[1–3] enables the controlled deposition of mass-selected ions onto surfaces. Recent advances in electrospray ionization (ESI) coupled deposition instruments now allow the formation of thin functional material layers using complex ions from the gas phase.[4–6] Collision-induced dissociation (CID) in the gas phase can be used to generate undercoordinated metal species. We deposited such ions onto layers on surfaces to create new model systems for DHI separation. Preserving ionic charge during deposition, supported by sequential deposition of cations and weakly coordinating anions, is critical for controlling the chemical reactivity of the deposits.[7]

A systematic investigation of the layers formed by co-deposition of the undercoordinated Ru complex with weakly coordinating anions (WCAs; $[B_{12}Cl_{12}]^{2-}$, $[PF_6]^-$) was conducted, with Reflection–Absorption Infrared Spectroscopy (RAIRS) providing detailed insight into the resulting layer compositions. Deposition of the Ru complex without stabilizing WCAs resulted in less abundant IR signals through degradation of the bipyridine ligand, whereas co-deposition with a WCA effectively suppressed this decomposition. To probe the “chemical availability” of the undercoordinated binding site within the layer, the prepared sample was exposed to CO atmosphere and the bound CO was detected by RAIRS. Stabilization by the WCA significantly enhanced CO adsorption at the metal center, which is apparently protected from undergoing undesired side reactions. Because this stabilization requires efficient ion–ion interaction, precise spatial overlap of the deposited cations and anions is essential. However, this approach revealed challenges because cation and anion beams often show a spatial offset at the surface.

To precisely assess the offset of two deposited types of ions across the surface, spatially resolved X-ray Photoelectron Spectroscopy (XPS) measurements were performed. The introduced methods are part of a currently developed procedure to ensure the best possible overlap of ion beams of sequentially deposited ions on surfaces.

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Mon 14:15–14:30: Contributed Talk – Maria Chiara Crimella

Deposition of charged microdroplets to quantify charge separation of salts in the ESI process

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Electrospray Ionization (ESI) is a widely used technique developed to transfer charged particles from solution into the gas-phase. We investigate how the charge of molecular salts in microdroplets changes dependent on ESI defining parameters (emitter diameter, ESI voltage, distance between the ESI capillary and the surface, flowrate, type of analyte and solution concentration). To do this we deposit microdroplets/ions onto a gold substrate under different vacuum conditions. We start with an atmospheric deposition of charged microdroplets, followed by a rough vacuum deposition (using an ion funnel chamber) and compare these results with an ion soft-landing (ISL) deposition of mass-selected bare ions under high-vacuum conditions of a mass spectrometer. Depending on the ions nature (atomic/molecular) we use different analytical methods (XPS, IR or NMR) to quantify differences in the ratio of anions to cations within the film generated on the gold substrate.

The results of atmospheric ESI depositions of salt solutions were found to be difficult to reproduce. We learned that the composition of the layers formed by collecting microdroplets emitted from the Taylor cone depends on the distance of the ESI capillary and the surface. Moreover, applied ESI voltage and flow rates of the solution have a major impact on the measured deposition current.

With this approach we try to generate insight into what properties salts must have to generate high ion currents through effective ionization.

Mon 14:30–15:00: Invited Talk – Martin Beyer

Hydrogen-Deuterium Exchange in Ionic Water Clusters

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Ionic water clusters in the gas phase provide deep insight into the mechanism of H/D-exchange reactions. Depending on the nature of the charge carrier, clusters $X^{+/-}(H2O)_{n-m}(D_2O)_m$ may or may not exhibit isotopic scrambling of H_2O and D_2O molecules to form HDO. Moreover, isotopic scrambling may occur only within a limited size range. The talk reviews key results in this field.

Honma and Armentrout studied the reactions of $H^+(H_2O)_n$, n = 1-4, with D_2O and $D^+(D_2O)_n$ with H_2O as a function of collision energy under single collision conditions.[1] At low energies, H-D exchange is efficient, but its contribution decreases with increasing energy. RRKM theory and ab initio calculations explain the observations consistently.

Sun et al. performed experiments a thermal energies, reacting D_2O with $H^+(H_2O)_n$, $(H_2O)_n^-$ and $O_2^-(H_2O)_n$, with $n \approx 30\text{-}50$.[2] Isotopic scrambling is clearly evident in the mass spectra by the elimination of HDO molecules from the cluster, which shifts the cluster mass from odd to even and even to odd, respectively. As expected, scrambling is efficient for $H^+(H_2O)_n$, but no H/D-exchange occurs in the anionic clusters that lack a mobile proton. Also many hydrated metal ions $M^+(H_2O)_n$, e.g. M = Cr, Fe, Co, Cu, Zn, do not exhibit scrambling.[3]

It is tempting to assing the occurrence of H/D-exchange and HDO formation to the presence of a proton donor or acceptor. However, Uggerud and co-workers showed that the situation is more subtle, since $NH_4^+(H_2O)_{n-m}(D_2O)_m$ clusters do not eliminate HDO.[4] In this case, the high proton affinity of ammonia keeps the excess proton from engaging in the Grotthus mechanism, which is needed for isotopic scrambling.

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Mon 15:30–16:00: Invited Talk – Linda Zhang

Distinct Lattice Responses and Adsorption Dynamics of Hydrogen Isotopologues in a Flexible Triazolate MOF

Linda Zhang [1,2], Richard Röß-Ohlenroth [3], Vanessa K. Peterson [4], Samuel Duyker [5], Cheng Li [6], Jhonatan Luiz Fiorio [7], Jan-Ole Joswig [7], Robert Dinnebier [8], Dirk Volkmer [3], Michael Hirscher [2,9]

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Separating gaseous mixtures of similar particles, such as hydrogen isotopes, is a premier challenge in modern separation technology. While conventional cryogenic distillation is energy-intensive, costs can be reduced by introducing selective porous sorbents like metal-organic frameworks (MOFs). In this work, we investigate the triazolate-based framework [$Mn(ta)_2$], which features a diamondoid-type topology. Unlike frameworks relying on open metal sites, [$Mn(ta)_2$] facilitates separation through isotopologue-induced structural dynamics within its confined pore-surface pockets [1].

Through *in situ* neutron powder diffraction (NPD), we observe a measurable lattice expansion upon gas loading that is uniquely more pronounced for H_2 than for D_2. This counterintuitive structural response is coupled with the identification of two distinct adsorption sites: Site 1 within the triazole pockets and Site 2 within the channels. At 60 K, D_2 occupies both sites simultaneously, whereas H_2 follows a sequential filling process, beginning with Site 1.

The isotope separation performance was characterized using cryogenic thermal desorption spectroscopy (TDS). A high D_2/H_2 selectivity of 32.5 is achieved at 60 K, representing one of the highest values reported for porous materials under similar conditions. This also allows for the enrichment of D_2 to 75% purity from a dilute 5:95 mixture in a single cycle. Given the commercial availability of the ligands and the scalability of the framework, [$Mn(ta)_2$] provides a realistic prospect for industrial-scale deuterium production.

[1] L. Zhang, R. Röß-Ohlenroth, V. K. Peterson, S. G. Duyker, C. Li, J. L. Fiorio, J. O. Joswig, R. Dinnebier, Dirk Volkmer, Michael Hirscher, *Nat. Commun.* **2025**, *16*, 5941.

Hydrogen isotope adsorption in V-doped MIL53(Al) using *in situ* EPR spectroscopy

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Metal-organic frameworks (MOFs) are well explored for their tunable properties like gas storage, band gap, catalysis, etc. Among them, flexible MOFs such as MIL53(Al) exhibits selectivity towards hydrogen isotope adsorption and separation at low temperature[1]. In this study, a vanadium-doped variant of MIL53 (Al) has been considered where the V^{4+} ions acts as paramagnetic probes to monitor the local structural change in the framework upon adsorption of molecular hydrogen. The *in situ* EPR spectroscopy clearly detect the presence of the narrow-pore (NP) and the large-pore (LP) phase for both hydrogen (H_2) and deuterium (D_2) isotopes, and notably an additional very-large-pore (VLP) phase that is only visible for D_2 adsorption at low temperatures[2]. These findings demonstrates that such a system provides a sensitive platform for probing hydrogen isotope adsorption and separation. Further understanding such adsorption processes could potentially contribute to the application of gas molecules separation and storage using metal-organic frameworks.

[1] J. Yeong Kim *et al.*, "Specific Isotope-Responsive Breathing Transition in Flexible Metal− Organic Frameworks," *J. Am. Chem. Soc*, vol. 142, p. 18, 2020, doi: 10.1021/jacs.0c04277.

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Mon 16:15–16:30: Contributed Talk – Akira Taguchi

H_2-D_2 separation in 8-membered ring zeolites (CHA, RHO, and LTA (4A)) at mild temperatures

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The separation of hydrogen isotopes is becoming increasingly important due to their expanding use in industrial applications and their role as potential energy carriers in prospective nuclear fusion reactors.[1,2] Porous materials, particularly metal-organic frameworks (MOFs), enable quantum sieving and are promising candidates for isotope separation with enhanced efficiency.[2] Because quantum sieving with cryogenic operating temperatures (< 77 K) significantly increase cost, achieving effective separation at relatively mild temperatures ($T_{exp.}$) is an another goal.

We have investigated the D_2/H_2 separation performance of 8-membered ring zeolites (Cs-CHA, RHO, and LTA(4A)) using thermal desorption/adsorption spectroscopy (TDS/TAS).[3] Cs-CHA and RHO type zeolites showed H_2 and D_2 desorption signals around 270 and 190 K, respectively, when exposing H_2-D_2 mixed gas (H_2/D_2 = 50.7/49.3, vol./vol) at 250 K ($T_{exp.}$) as TDS spectra started from 77 K was shown in Figure 1. The D_2/H_2 selectivity ($S_{D2/H2}$) for this high temperature desorption reached 1.42 and 1.36, respectively, although the desorbed amount remained below 1.0 mmol g^{-1}.

Since 8-membered ring zeolites are known to be difficult to characterize by conventional sorption isotherms, we employed our TAS study, which monitors pressure changes during a temperature ramp in a closed system. The TAS measurements confirmed hydrogen adsorption in CHA- and RHO-type zeolites at temperatures consistent with the corresponding TDS desorption phenomena.

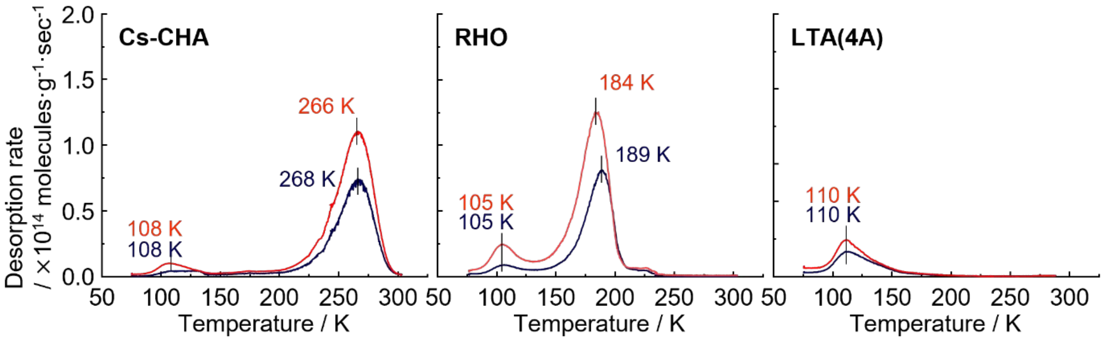

Figure 1: TDS spectra of Cs-CHA ($Cs_{8.8}K_{2.9}[Si_{24.9}Al_{11.1}O_{72}(OH)_{0.6}]$, RHO ($Na_{4.7}Cs_{3.1}[Si_{40.2}Al_{7.8}O_{96}]$), and LTA(4A) ($Na_{5.8}K_{5.9}[Si_{12.1}Al_{11.9}O_{48}]$) started from 77 K ($T_{exp.}$= 250 K).

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Mon 16:30–17:00: Invited Talk – Irena Senkovska

Particle size tuning of responsive MOFs as a tool to achieve efficient gas separation performance

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Flexible metal-organic frameworks (MOFs) that show reversible guest-induced phase transitions between closed and open pore phases have enormous potential for highly selective, energy-efficient separations because they can selectively respond to external stimuli, adapting their pore size triggered by adsorption-induced gating or breathing.[1]

Despite recent studies that have provided some guidelines for understanding and designing structural flexibility for controlling gate opening by chemical modification of the secondary building units, currently, there is no established strategy to design a flexible MOF showing selective gated adsorption for a specific guest molecule.

In this contribution, we demonstrate, on the example of DUT-8 MOF, that the selectivity in the adsorption-induced gate-opening can be tuned, altered, and even reversed using particle-size engineering.

DUT-8 consists of paddle wheels, 2,6-naphthalenedicarboxylate linkers, and 1,4-diazabicyclo(2.2.2)octane pillars forming a primitive cubic net. It is capable to reversible phase transition, transforming the material between non-porous and porous states, which is manifested in the “gating type” adsorption isotherms for specific adsorptives.

DUT-8(Ni) is able to discriminate between CO_2 and CH_4 in the mixture of these gases at room temperature, leading to near-perfect selectivity.[2] It is also able to isotopolog-selective switching, demonstrating D_2 over H_2 selective responsivity as well as preferable adsorption of D_2 over H_2.[3]

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Day 2 — 24 March 2026

Tue 09:00–09:45: Keynote Talk – Volker Derdau

Hydrogen Isotope Exchange of Biologicals - a Real Challenge

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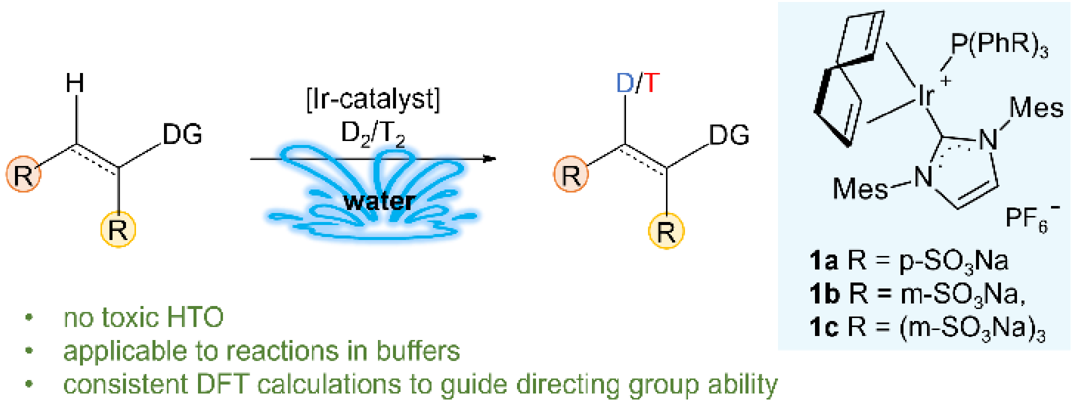
Isotopic labeling of organic compounds is crucial for advancements in life sciences and is extensively utilized in drug discovery. While isotopic labeling is widely applied to small molecules, research on isotopically labeled biologics such as peptides, antibodies, or enzymes remains less developed, despite the increasing prevalence of these larger biologics in the pharmaceutical industry as transformative treatments for patients. We report on the development of Hydrogen Isotope Exchange (HIE) reactions with deuterium or tritium gas in buffers.[1,2,3]



1a R = p-SO_3Na
1b R = m-SO_3Na,
1c R = (m-$SO_3Na)_3$

- no toxic HTO
- applicable to reactions in buffers
- consistent DFT calculations to guide directing group ability

Figure 1: Iridium catalyzed HIE reactions in aqueous buffers.

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[3] E. Martinelli, R. Weck, S. Güssregen, and V. Derdau* submitted.

The Role of Protons in Electrocatalysis

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The interplay between electrons, protons, and substrate molecules governs the efficiency and selectivity of electrocatalytic reactions. In most cases, electron transfer initiates the reaction, for example through changes in oxidation state, followed by substrate binding and subsequent protonation events, either of the substrate itself or of nearby functional groups. The sequence and kinetics of these elementary steps are critical determinants of catalytic selectivity.

In electrocatalysis, electrons are supplied directly by the electrode, whereas substrate binding and proton transport typically occur through the electrolyte. Consequently, simultaneous accessibility to both electrons and protons is a key design principle for efficient electrocatalytic systems.

In this talk, I will analyze on several examples the interplay between charge transfer and catalytic transformation in the oxygen and hydrogen reduction reactions using in situ vibrational spectroelectrochemistry. Different electrocatalytic strategies based on enzymatic[1], molecular[2], and material-based[3] catalysts will be evaluated. Across all systems, particular emphasis will be placed on the role of protonation events in governing reaction pathways and selectivity.

[1] F. Kruse, A. D. Nguyen, J. Dragelj, J. Heberle, P. Hildebrandt, M. Mroginski, I. M. Weidinger *J. Am. Chem. Soc*. **2021** *143*, 2769-2776.

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[3] M. Borelli, C. J. Querebillo, D. L. Pastoetter, T. Wang, A. Milani, C. Casari, H. K. Ly, F. He, Y. Hou, C. Neumann, A. Turchanin, H. Sun, I. M. Weidinger, X. Feng *Angew. Chem. Int. Ed.* **2021** *60*, 18876–18881.

Tue 10:15–10:30: Contributed Talk – Kwangjin An

Catalyst Design for Liquid Organic Hydrogen Carriers (LOHCs)

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Liquid organic hydrogen carriers (LOHCs) represent a safe and efficient medium for reversible hydrogen storage, enabling practical deployment of hydrogen energy technologies. However, developing catalytic systems that allow low-temperature, reversible dehydrogenation with high stability remains a critical challenge. In this study, we present a comprehensive approach to designing Pd-based catalysts by tailoring the physicochemical properties of metal–support interfaces. Through rational modification of oxide supports—via incorporation of promoters, defect engineering, and structure control—we systematically modulate electronic interactions and hydrogen-related surface behaviors. Charge transfer phenomena, surface acid–base tuning, and hydrogen spillover are leveraged to promote reversible hydrogen activation and facilitate dynamic adsorption–desorption processes.[1-3] This integrative catalyst design strategy offers insights into achieving both efficient hydrogen release and storage in *N*-heterocyclic LOHC systems. Our findings underscore the potential of support engineering as a general platform to realize practical, low-temperature reversible LOHC processes using earth-abundant catalytic materials.

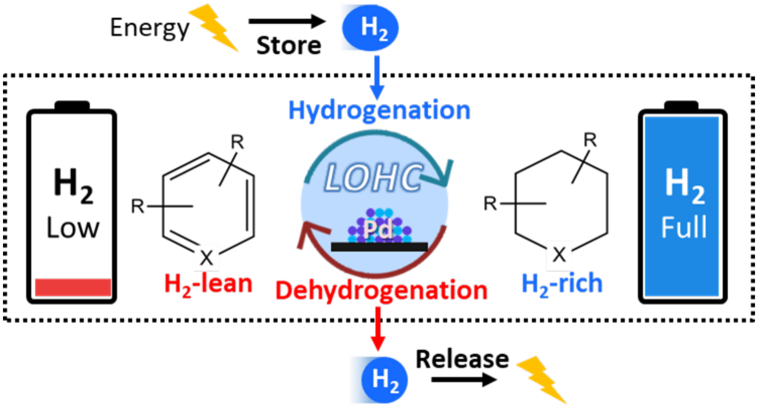

Figure 1: Schematic diagram of effective catalyst design for LOHC system.

[1] J. Lee, B. G. Park, K. Sung, E. Nam, H. Lee, J. W. Han, and K. An, *ACS Catal.*, **2023**, *13*, 13691-13703.
[2] B. G. Park, J. Lee, Y. Lee, H. Lee, J. Kim, E. Nam, J. -S. Bae, J. W. Han, and K. An, *ACS Catal.* **2025**, 1563-1575.
[3] H. Lee, Y. Kim, H. Ryou, J. Kim, D. Oh, E. Nam, J. Kim, S. Lee, J. Bae, C. Hur, J. -S. Bae, B. G. Park, J. Han, H. Sohn, and K. An, *ACS Catal.* **2025**, *15*, 13243-13259.

Tue 11:00–11:30: Invited Talk – Cornelius Fischer

Hydrogen Isotope (^1H, ^2H, ^3H) Interactions With Microporous Materials: Experimental and Analytical Insights

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Efficiently separating hydrogen isotopes is necessary for a variety of applications. Consequently, several strategies employing advanced materials have recently been explored. The issue appeared to be largely settled by using microporous, nanostructured materials, either 2D[1] or 3D pore networks[2] — as the approach is conceptually sound, theoretically fairly well understood, and feasible in principle in terms of materials science. Experimentally, this task has been accomplished using protium and deuterium. The vexing problem of working with radioactive tritium was tacitly subsumed under this conceptual framework and dismissed as a rather technical problem, offering limited mechanistic insights.

Here, we discuss experimental approaches that enable the study of $^{1,2,3}H$ isotope mixtures.[3] We present an overview of the results of separation experiments using proton-conducting membranes, as well as the isotope-specific sorption efficiencies of microporous materials. Important candidates include zeolites[4] and metal-organic frameworks (MOFs). Another aspect of our investigations is the stability of the materials used. Initial interpretations of possible material alteration during tritium exposure focused on radiation damage; however, interest in the tritiation of material surfaces as a decisive alteration mechanism is growing.[5] Overall, we are reviewing the recent separation results of binary and ternary isotope mixtures and addressing the issue of substrate deterioration.

[1] M. Lozada-Hidalgo, S. Hu, O. Marshall, A. Mishchenko, A. N. Grigorenko, R. A. W. Dryfe, B. Radha, I. V. Grigorieva, A. K. Geim, *Science* **2016**, *351*, 68-70.

[2] J. Teufel, H. Oh, M. Hirscher, M. Wahiduzzaman, L. Zhechkov, A. Kuc, T. Heine, D. Denysenko, D. Volkmer, *Advanced Materials* **2013**, *25*, 635-639.

[3] A. Becker, H. Lippold, J. P. Bäcker, D. Belder, C. Fischer, *Radiochimica Acta* **2024**, *112*, 231-237.

[4] A. Becker, H. Lippold, M. Hirscher, C. Fischer, *arXiv preprint arXiv:2510.03333* **2025**.

[5] A. Becker, G. Zeller, H. Lippold, I. Eren, L. R. Müller, P. Chekhonin, A. B. Kuc, M. Schlösser, C. Fischer, *arXiv preprint arXiv:2506.20304* **2025**.

Tue 11:30–11:45: Contributed Talk – Alexander Feige

Electron Diffraction as an Alternative to Neutron Methods for Hydrogen Isotope Identification

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Distinguishing between hydrogen isotopes using diffraction methods has traditionally relied on the pronounced differences in neutron scattering lengths in neutron powder diffraction experiments, which usually average over all particles in a complete powder sample and are often only available in larger research facilities.[1] In this work, I will show that hydrogen and deuterium atoms can also be unambiguously distinguished using electron diffraction data, based on datasets of KH_2PO_4 and KD_2PO_4. Despite the similar electron scattering factors of these isotopes, precise refinement of atomic displacement parameters reveals distinct thermal motions, reflecting the isotopes' differences in atomic mass. Compared to neutron powder diffraction, the advantage of this methodology is that it is readily accessible to any standard laboratory equipped with a transmission electron microscope. The results represent a significant advance towards routine differentiation of hydrogen and deuterium by diffraction alone – eliminating the need for sample shipment to nuclear reactors or spallation sources.

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Tue 11:45–12:00: Contributed Talk – David Egloff

From Experience to Engineering:
The Evolution of Safe and Refined Tritium Handling

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For the labeling of compounds with tritium, either specific tritiating agents or, still predominantly, tritium gas itself is used today. Its radioactivity makes it a very powerful tool for the research and development of human and animal pharmaceuticals and crop protection agents. At the same time, this property poses significant constraints in terms of safety and regulation compared to its isotopes hydrogen and deuterium[1].

RC Tritec (then called Radium-Chemie Teufen) was among the first companies to work with tritium when it became commercially available in the late 1950s[2]. It was used to develop an alternative for 226Ra activated phosphorescent paints, which had become known to be highly hazardous due to their strong radiation. Two decades later, RC Tritec used its accumulated knowledge about tritium to label compounds for the pharmaceutical industry.

In those days, tritium gas was often shipped in glass vessels and chemical reactions were performed using handling systems made of glass[3]. The inherent brittleness of glass and the increase in internal pressure due to the formation of the decay product 3He were among the risks that had to be addressed.

Today, tritium handling systems are highly engineered stainless-steel installations that ensure safe and precise handling of tritium by minimizing exposure, enabling exact control of pure gas and reducing the release of tritium into the environment. In addition, different getter materials, such as depleted uranium, have simplified the safe transport and storage of this radioactive gas.

Driven in part by the rapid advancement of fusion research, the development of even more advanced and safer tritium handling systems is progressing. Consequently, development efforts are currently being intensified not only at RC Tritec, e.g. in the fields of getter materials, diffusion barriers and tritium recycling.

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Tue 12:00–12:30: Invited Talk – Genrich Zeller

Raman Spectroscopy and Microscopy of Tritiated Samples

Genrich Zeller, Deseada Díaz Barrero, Robin Größle, Alexander Marsteller,
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Tritium analytics is required across a broad range of experimental and technological fields. The closed tritium circulation loop of the Karlsruhe Tritium Neutrino (KATRIN) experiment is a key example thereof.[1] Fuel-cycle accountancy, detection of tritiated compounds that contaminate fuel[2], characterization of tritium bound to surfaces/functionalized materials are other examples needing reliable tritium analytics. In this context, research on tritiated graphene is a growing field, with concepts for future neutrino experiments and fusion fuel-cycle hydrogen isotope separation.[3,4]

Raman spectroscopy is a versatile, non-invasive tool applicable to tritium in gaseous, aqueous, and solid-bound forms. This talk presents recent Raman spectroscopy/microscopy results gathered at the Tritium Laboratory Karlsruhe (TLK), covering mainly the analysis of tritiated gas mixtures and tritium-graphene interactions.

For tritiated gases, laser Raman spectroscopy is employed for continuous, accurate, in-line composition monitoring of hydrogen isotopologues in the inner tritium loop of KATRIN, demonstrating demanding < 0.1 % precision over multi-year timescales.[5] Intensity calibration and validation measures required to maintain high trueness during KATRIN operation are presented.

Based on over two decades of Raman expertise combined with profound tritium process needs, TLK developed a process-oriented Raman system, now available to the public via an industry partner. For tritium bound to graphene, a tritium-compatible, inhouse-built confocal Raman microscope is used, leveraging established expertise in safe tritium handling and calibrated Raman spectroscopy.[6] Raman mapping is used to track spatially resolved signatures of tritium-induced modifications, focusing on defect-related features consistent with sp^3-type contributions from C-T bonding. Their evolution over time, spatial homogeneity, and response to thermal treatment provide valuable insight into reversible versus persistent defect formation.[7]

Together, these case studies illustrate the complementary scope of Raman methods for tritiated samples, from process-driven, easy-to-operate systems to highly specialized research-grade devices for spatially resolved characterization of tritium-graphene interactions in solids.

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Tue 13:30–14:00: Invited Talk – Olga García Mancheño

Late-stage Photocatalytic Hydrogen Isotope Exchange and H-isotope Effects Towards Selective Reduction Reactions

Olga García Mancheño,† Martin Stinglhammer, Jan-H. Kuhlmann, Elisa Martinelli, Stefania Perulli, Martin Sandvoss, Christian Mück-Lichtenfeld, Volker Derdau, Martín Aleksiev, Susumu Saito

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Deuterium-labeled compounds are emerging tools in drug discovery, since deuteration often improves the pharmacokinetic and/or toxicity profile of drugs,[1] Several strategies for the synthesis of deuterated compounds have emerged, many of them relying on carbonyl reduction, hydrodeuteration of olefins, or hydrogen isotope exchange (HIE).[2],[3] However, they yet often result in multiple position- or only partly labeled compounds, for which precision deuterium labeling procedures are still in high demand.

Along these lines, we recently developed a highly regioselective visible light photoredox-catalyzed hydrogen isotope exchange (HIE) of benzylic positions in both simple and complex molecules.[4] The process follows a dual catalytic approach using an acridinium photocatalyst in combination with a thiol-based hydrogen atom transfer catalyst, while the use of D_2O as an isotope source ensures operational simplicity and cost-effectiveness. In this lecture, key mechanistic insights and the utility of the reaction on the late-stage site-selective HIE of several natural benzylic compounds and drug derivatives will be discussed. Finally, a different approach for the site-selective deuteration vs. hydrogenation of carboxylic acids based on metal-catalyzed reduction will be presented.[5]

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Tue 14:00–14:15: Contributed Talk – Hannah Buttkus

Hydrogen Isotope Effects Used to Reveal Vibrational Signatures of a Microsolvated Hexafluorophosphate Anion

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Hexafluorophosphate (PF_6^-), widely used in lithium-ion batteries and known to release biologically damaging hydrofluoric acid upon hydrolysis, has recently been detected in environmental waters.[1,2] Molecular-level insight into its interactions with solvents like water or 1,1,1,3,3-hexafluoroisopropnaol (HFIP), which catalyze PF_6^- hydrolysis, is therefore crucial for understanding solvation behaviour and for providing reliable input to computational simulations.[2]

In this ongoing study, we investigate how HFIP and its isotopologues influence the microhydration of PF_6^-. The complexes $PF_6^-(HFIP)_x(H_2O)_y$ are systematically investigated by IR photodissociation spectroscopy in the spectral region between 800 – 4000 cm^{-1} and assigned using electronic structure calculations.

In single-solvent complexes, HFIP and H_2O each engage in weak hydrogen bonding with PF_6^-, as indicated by O-H stretching frequency shifts $\Delta\nu(\mathrm{OH})$ of less than 200 cm^{-1}. Additional HFIP molecules continue to engage in ionic hydrogen bonding, while H_2O molecules prefer to form an intramolecular hydrogen-bonded network on one side of the anion, whereas HFIP primarily engages in ionic hydrogen bonding. In mixed-solvent $PF_6^-(HFIP)(H_2O)_x$ (x = 1-5) complexes, HFIP is incorporated into the hydrogen-bonded network, cooperatively strengthening the inter-solvent hydrogen bond ($\Delta\nu(\mathrm{OH})$ = 873 cm^{-1}) while weakening the PF_6^- - water interaction ($\Delta\nu(\mathrm{OH})$ = 91 cm^{-1}). In $PF_6^-(HFIP)_x(H_2O)$ (x = 1-3) complexes, additional HFIP molecules weaken the HFIP - water hydrogen bond yet simultaneously promote solvation-enhanced proton transfer between PF_6^- and water, offering first molecular evidence for the onset of HFIP-catalyzed PF_6^- hydrolysis.

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Tue 14:15–14:30: Contributed Talk – Erik Butenschön

What ^{1}H & ^{2}H NMR Reveals About Enzymatic PET-Degradation

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With global plastic production steadily increasing,[1] enzymatic recycling of polymers such as polyethylene terephthalate (PET) is being explored as a promising, energy-saving alternative.[2] Understanding the mechanisms underlying this biocatalytic recycling process may enable rational protein engineering, thereby launching a new and more efficient technical opportunity to enhance the extent of plastic waste recycling.

Advances in Nuclear Magnetic Resonance (NMR) spectroscopy have enabled the study of kinetics, dynamics, and structural features of enzyme-substrate binding sites. Using liquid-state ^{1}H & ^{2}H NMR, we were able to investigate quantitative product formations of enzymatic PET-degradation under various conditions, without the need for calibration curves (Fig. 1A & B). Under static conditions, ^{2}H can be used as a probe for dynamics due to its quadrupolar coupling. Utilising this, we were able to investigate the dynamics of PET (Fig. 1C) as well as of the aromatic amino acids present in the enzyme.

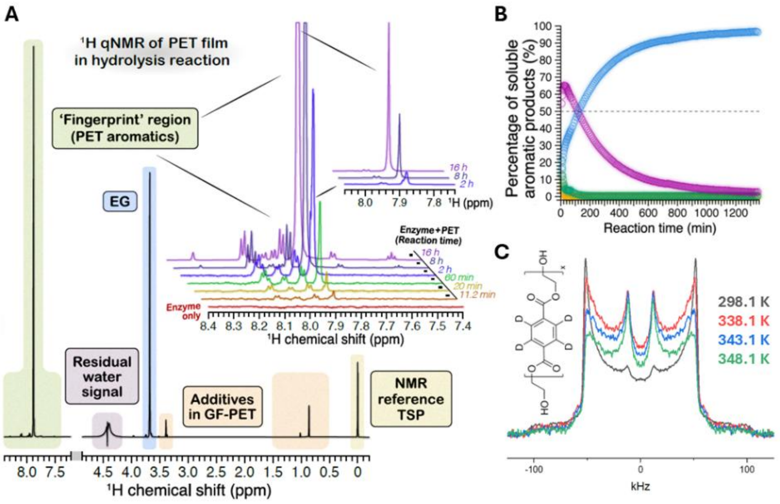

Figure 1: A) Using liquid-state ^{1}H NMR with solvent suppression, build-up and degradation of soluble products from enzymatic PET-degradation can be measured. B) Their signal integrals give insight into product formation and mechanistic understanding. C) Static solid-state ^{2}H Pake pattern of selectively labeled ^{2}H-PET at various temperature, highlighting a change in dynamics.

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Integrated Chemical Microlaboratories: A Key Technology for Automated, Safe, and Sustainable Reaction Processing

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The miniaturisation of chemical functional elements, such as reactors and analytical components, enables the development of integrated chemical microlaboratories capable of monitoring and controlling chemical transformations in real time. These advantages are particularly relevant for the synthesis of tritium-labelled compounds, where minimised reagent inventories, enhanced containment, and precise process control are essential for safety and regulatory compliance. Within lab-on-a-chip-like microsystems, both classical batch synthesis in microreactors and continuous-flow synthesis can be realised.

Digital microfluidics (DMF) offers a versatile platform for microbatch synthesis through automated droplet manipulation under closed conditions, enabling seamless integration with powerful analytical techniques for label-free, sensitive, and nondestructive reaction monitoring. In radiochemical applications, droplet-based microfluidic systems provide intrinsic containment, reduced radioactive waste generation, and remote operability. Although the complete functional integration of continuous-flow lab-on-a-chip systems remains challenging, modularisation within a microfluidic breadboard architecture represents a promising alternative. This strategy simplifies implementation, promotes standardisation, and enables the reconfigurable integration of microreactors and analytical modules, such as chip-based HPLC and miniaturised electrospectrochemical systems tailored to tritium chemistry. Together, these developments outline a practical and scalable pathway towards flexible, automated, and inherently safer microlaboratories for next-generation tritium-labelled synthesis and radiochemical processing.

Tue 15:30–16:00: Invited Talk – Jörg Meyer

New Insights into the Volume Isotope Effect of Ice Ih from Polarizable Many-Body Potentials

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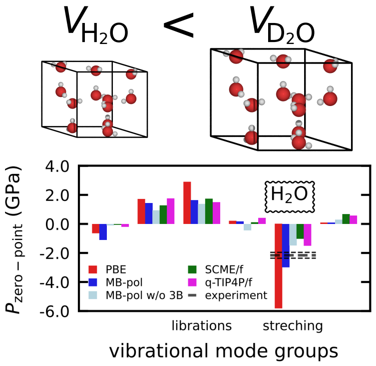

In crystalline phases of water nuclear quantum effects manifest themselves quite prominently in macroscopic thermodynamic properties, like for example phase transition enthalpies [1] or the density change at low temperatures [2] . The latter is called the volume isotope effect (VIE). In most materials, substitution with a heavier isotope results in a smaller volume at temperatures approaching the absolute zero. Handwavingly, in a classical picture, this can be rationalized by the smaller vibrational amplitude ascribed to a heavier nucleus experiencing the same chemical interaction potential at the same temperature. In contrast, the molar volume of the D_2O isotopologue of ice Ih is 0.1% larger than that of its H_2O counterpart, which is called *anomalous* VIE. Earlier computational studies established a link to the zero-point energy of intra- and intermolecular vibrational modes (phonons). However, even the most elaborate force fields developed from basic principles yielded a normal VIE in clear contradiction to experiments. Furthermore, DFT calculations with various exchange-correlation functionals have been struggling to get close to the experimental data. This made it difficult to determine which contributions to the interaction potential result in what effects on the different types of phonon modes and impossible to identify which of them are responsible for this subtle effect. Motivated by recent high-precision neutron diffraction experiments [3], here we present a computational study based on the quasi-harmonic approximation [4]. We focus on recently developed polarizable many body potentials [5,6] and find that one of them, MB-pol [6], yields the anomalous VIE in good agreement with the most recent high-resolution neutron diffraction measurements – better than many density functionals. We further scrutinize the interaction potentials by decomposing the zero-point pressure into contributions from different vibrational mode groups. This allows us to confirm the remarkable performance of MB-pol by comparing to a hitherto unconsidered “independent” benchmark value for the intramolecular stretching modes of H_2O ice Ih obtained from Raman spectroscopy data. According to MB-pol, the librational and stretching are the most important phonon modes responsible for the anomalous VIE, mitigated by short-range three-body effects. This prediction is experimentally verifiable. Our study thus goes one step further towards a deeper understanding of hydrogen-bonding in this most ubiquitous and important system.

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Tue 15:30–16:00: Invited Talk – Jörg Meyer

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Tue 16:00–16:15: Contributed Talk – Muhammad Fernadi Lukman

Local Structure Insight of Flexible Cu^{2+} doped ZIF-8 and Its Application to Hydrogen Isotopologues Detection

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The doping of Cu^{2+} to the Zn^{2+} site on the ZIF-8 framework has been investigated by a combination of multifrequency EPR techniques aided by quantum-chemical calculations [1] (as illustrated in Figure 1). X-band continuous wave (CW) EPR spectra exhibit the presence of Cu^{2+} species with spin Hamiltonian parameters consistent with a distorted tetrahedral geometry, at a crossroad between D_{4h} and D_{2d} symmetry. Such a constraint in the geometry is amenable to the framework incorporation of Cu^{2+} ions in the MOF lattice. The ENDOR spectroscopy reveals the presence of strongly coupled ^{14}N nuclei, dominated by a large Fermi contact term, pinpointing the formation of a σ-bond between Cu and N ligands of the linkers. This provides unequivocal evidence for framework substitution of Cu^{2+} at Zn^{2+} sites. In addition, the flexibility of such a framework can be traced through changes in the Cu^{2+} local environment on the advent of "gate opening" in response to the N_2 gas adsorption [2]. Ultimately, we have implemented the *in situ* hyperfine spectroscopy setup as a novel approach in this field [3] with comparable measurement conditions and results as for the already established (thermal desorption spectroscopy) TDS method. Furthermore, *in situ* electron spin echo envelope modulation (ESEEM) extends the high-resolution advantage of ESEEM to explore the pore fillings by D_2 and HD during the adsorption and desorption processes. In this context, *in situ* ESEEM measurements were implemented for the ZIF-8 system as a first application example employing two distinct spin probes with different perspectives: Cu^{2+} at framework sites (as comprehensively investigated through multifrequency EPR and DFT predictions) and TEMPO radicals within the pores. The *in situ* ESEEM results for both probes successfully mapped the D_2 or HD density in the pores of ZIF-8 during the adsorption-desorption processes, in agreement with previous volumetric adsorption data.

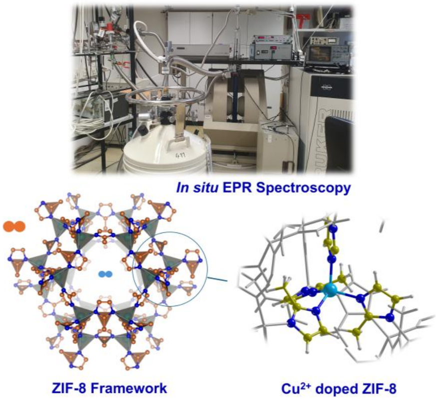

Figure 1 In situ EPR spectroscopy setup at Leipzig University (Top), illustration of the ZIF-8 framework for hydrogen isotopes adsorption (bottom left) and local structure of Cu^{2+} doped into the ZIF-8 (bottom right).

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Tue 16:15–16:30: Contributed Talk – Nils Hertl

Mode selectivity in electron promoted vibrational relaxation of chemisorbed hydrogen on molybdenum and tungsten surfaces

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Vibrational relaxation induced by electron-hole pair (EHP) excitations is a common phenomenon in gas-surface experiments on metallic surfaces[1–4]. Specific adsorbate vibrational degrees of freedom can be more strongly coupled to EHPs at metal surfaces than others, which opens an opportunity for mode-selective energy transfer processes that can activate chemical dynamics.

To promote mode-selective chemical reactions at solid interfaces a detailed understanding of the coupling of the individual vibrations of adsorbates with the electrons and phonons of the metal substrate is essential. To shed light on the mechanisms involved in energy transfer processes present in gas-surface systems, we study adsorbed hydrogen on single crystalline surfaces.

We calculated the linewidths of vibrational modes of hydrogen and deuterium adsorbed on the (100) and (110) surfaces of molybdenum and tungsten via first-principles first-order perturbation theory based on Density Functional Theory (DFT) [5, 6]. Our results show a strong mode dependency on the electron-driven relaxation rates of the vibrations. For the vibrations with a Fano-lineshape [7], our predicted lifetimes are in good agreement with experiments, indicating that the relaxation of those vibrations is dominated by EHP excitations [8]. Our calculated linewidths show a strong coverage dependence, decreasing with increasing coverage. Hence, EHP excitation is the dominant energy-transfer mechanism between hydrogen and pristine metal surfaces, but other channels for energy dissipation, such as adsorbate–adsorbate interactions, may become more significant on metal surfaces densely covered with hydrogen.

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Tue 16:30–17:00: Invited Talk – Alexandra Becker

Preparation and Characterization of Solid Low-Activity Tritium-Loaded Samples

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Tritium plays a key role in a wide range of research fields, such as direct neutrino mass experiments[1] and the fusion fuel cycle[2]. In many of these applications, tritium is incorporated into solid materials for purposes such as separation, retention, storage, or use as calibration sources.[3, 4] As research in these fields advances, the demand for reliable characterization and quantification of tritium in solid samples continues to grow. Examples of such solid tritium-interfacing materials include graphene, which is of interest for hydrogen isotope separation[5], and thin metal layers, used as tritium getters[6]. These metal layers may additionally serve as calibration sources for radiation detection techniques such as beta-induced X-ray spectroscopy (BIXS).[7]

For the use in research, these samples need to be well-characterized. However, characterization methods can be difficult to access, due to the radioactive nature of tritium, especially concerning surface contamination and outgassing from substrates. Additionally, volatile surface activity complicates the handling of solid samples for the aforementioned detector systems, making suitable decontamination methods as well as quantification techniques necessary.

One well-established tritium quantification method is liquid scintillation counting (LSC).[8] As it is usually performed with liquid tritium samples, measuring solid samples and contamination from outgassing presents some unique challenges, e.g., the interaction between the LSC cocktail and the sample being limited to the sample surface.

Figure 1: Schematic of tritium loading in metal samples (left) and on graphene (right).

Within this work, a potential strategy for the preparation (cf. Figure 1) and decontamination of low-activity solid tritium-loaded samples is presented. This includes a more direct approach to measuring the contamination of storage containers, caused by outgassing, as well as a strategy to measure loosely bound surface contamination.

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Day 3 — 25 March 2026

Wed 09:00–09:45: Keynote Talk – Melanie Schnell

H-isotope dependent effects revealed with high-resolution molecular spectroscopy

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Rotational spectroscopy is a coherence technique, which is used to determine the structures of molecules and molecular complexes in the gas phase in great detail. The structural information that can be deduced from the spectroscopic data provides an unprecedented molecular view on chemical processes, such as solvation and molecular recognition. H/D isotope exchange can have a tremendous influence on these topics, for example via its differences in vibrational zero-point energies. In this lecture, some examples of (micro-)solvation and molecular recognition will be addressed.

Starting with smaller systems, the HCl-Ne dimer case[1] will be discussed, where H/D isotope exchange changes the intermolecular vibrational dynamics and thus the overall electric dipole moments of the respective dimers.

In another series of studies, we exploited nuclear quadrupole coupling effects that reveal themselves in characteristic, additional line splittings in rotationally resolved spectroscopy. These splittings also depend on the electronic environment of the quadrupolar nucleus and thus provide valuable information about its bonding situation. Recently, this has been exploited to investigate water-driven dissociation of a single HCl molecule. It was possible to precisely determine how many water molecules are needed for HCl to dissociate[2]. In a related study, hydration of ethanolamine was investigated[3], and its nuclear quadrupole coupling pattern of the ^{14}N atom of the amino group was found to be strongly correlated with the strengths of the hydrogen bonds that the amino group was involved in the water network. These results further establish nuclear quadrupole coupling as a sensitive probe for the electronic environment.

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Wed 09:45–10:15: Invited Talk – Anne B. McCoy

Deciphering spectral signatures of proton delocalization in hydrogen-bonded complexes

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In this talk, we will explore the use of a variety of theoretical and computational approaches for exploring proton delocalization in complexes complexes that are held together by strong ionic hydrogen bonds. Of particular interest are complexes containing of hydroxide and hydronium ions with several water molecules. Over the years, the combination of theoretical work and experimental studies of these complexes have provided important insights into proton mobility in the bulk. The advantage of focusing on the smaller systems is that they allow direct comparisons to be made between experiment and calculation. In addition to providing assignments to peaks in the spectra, work on these systems provides insights into the underlying ionic hydrogen bonds. In these systems the cooperative nature of the hydrogen bond that are formed leads to large changes in the strengths of the ion-water interactions as more water molecules are introduced, and this, in turn, has a large effect on the spectroscopy. This work employs an array of theoretical and computational approaches, ranging from analysis of the couplings of the vibrations at the harmonic level through analysis of the wave functions using diffusion Monte Carlo approaches. The work is motivated by experimental studies of the vibrational spectra of these complexes. Recent work in the development of potential surfaces for hydroxide-water complexes will also be discussed.

Vibrational Signature of Shared Hydron in Deprotonated HFIP Dimer and Trimer

Milena Barp, Tatiana C. Penna, Jiaye Jin, Knut R. Asmis

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1,1,1,3,3,3-hexafluoroisopropanol, HFIP, is a protic organic solvent that finds broad application in several chemistry fields, from life sciences to material synthesis.[1] Many of its applications are related to its hydrogen bond (HB) donor ability[2] and to the promotion of proton transfer reactions, both associated to the stability of its conjugated base,[3] $(CF_3)_2CHO^-$. However, only a few experiments have interrogated these properties on a molecular level.[4] In this work, we used the powerful tool kit of cluster science and conduct cryogenic ion vibrational spectroscopy experiments to investigated the deprotonated HFIP dimer and trimer, building a model system in a bottom-up approach to understand the negatively charged chemical species involved in proton transfer reactions.

For the deprotonated HFIP dimer, the motion of the shared proton along the OO coordinate in the $[RO^- \text{-} H^+ \text{-} OR^-]$ moiety is characterized by a vibrational transition around 892 cm^{-1} where more than one band is found, while the free OH of HFIP is found at 3668 cm^{-1}. When H^+ is substituted by D^+, the experiments conducted at the Free Electron Laser of the Fritz-Haber-Institute confirm the shared deuteron stretch around 620 cm^{-1}, a ν_H/ν_D of 1.44, in excellent agreement to the theoretical 1.41 prediction. For the trimer, a greater delocalization of the negative charge over another OH moiety, $[RO^- \text{-} H^+ \text{-} OR^- \text{-} H^+ \text{-} OR^-]$, leads to a reduction of the vibrational shifts, *i.e.* an increment of the transition energy, and the two proton motions are now characterized by two broad bands (FWHM = ~150 cm^{-1}), one with lower intensity, centered at 1710 cm^{-1} and a more intense band centered at 2566 cm^{-1}. The large shifts (> 1000 cm^{-1}) reveals again the characteristic strong HB formed between deprotonated HFIP and a neutral solvent molecule, highlighting both the stability of the conjugated base as an excellent HB acceptor and the acidic nature of the proton in the neutral HFIP, that acts as a HB donor and serve as medium for proton transfers.

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Graphene and its interactions with protons and hydrons

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An ideal proton exchange membrane should only permeate protons and be leak tight for fuels. Graphene is impermeable to water and poorly conducting to protons. Here, we chemically functionalized monolayer graphene to install sulfophenylated sp^3 dislocations by diazotization. Selective to protons, transmembrane areal conductances are up to ~50 S/cm^2, which is ~5000 fold higher than in pristine graphene. Mounted in a direct methanol fuel cell, sulfophenylated graphene resulted in power densities up to 1.6 W/mg or 123 mW/cm under standard cell operation (60 °C), a value ~two-fold larger than micron-thick films of Nafion 117. The combination of sp^3 dislocations and polar groups, therefore, allow the creation of hydrophilic ion paths through graphene and unveils a novel route to rationalize transmembrane hydron transport through 2D materials.

Effects of Mechanical Strain and Local Curvature on Hydrogen Isotope Selectivity in Graphene Membranes

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Atomically thin graphene is a promising platform for hydrogen isotope separation due to its impermeability to most atoms and selective proton permeation.[1] Experiments by the Lozada-Hidalgo[2] group have reported permeation velocity ratios of approximately $H^+/D^+ \approx 10$, $H^+/T^+ \approx 30$, and $D^+/T^+ \approx 2$, which demonstrate isotope-dependent selectivity.

Under environmental conditions, graphene membranes are not perfectly flat.[3] Thermal fluctuations and hydration forces induce intrinsic in-plane and out-of-plane corrugations. Experimental studies have shown that high-proton-conductivity regions are observed near ripples, wrinkles, and strained regions, indicating that local lattice deformation is a key factor in hydrogen isotope transfer.[4]

In this work, we investigate how controlled biaxial tensile strain (1–5%) and local curvature influence isotope selectivity (H^+, D^+, T^+) in graphene membranes. Moderate tensile strain enlarges interatomic spacing and reduces the activation barrier for proton transfer, while local curvature modulates the barrier depending on its out-of-plane deformation. The results provide insight into how biaxial strain and ripples can modulate proton conductivity and isotope separation performance in graphene membranes.

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Wed 11:45–12:00: Contributed Talk – Dario Calvani

Enhanced and Selective Unidirectional Proton Transport via Covalent Benzenesulfonic Functionalized Nanoporous and Pristine Graphene

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A fundamental understanding of proton transport through graphene and graphene nanopores is essential for developing innovative two-dimensional proton exchange membranes. We computationally explore ways to enhance proton transport features using a combination of ReaxFF Molecular Dynamics, Metadynamics, and Density Functional Theory (DFT). We identified consistent improvements in proton permeability, in terms of activation barrier and selectivity, for the benzenesulfonic functionalized graphene nanopore and pristine graphene compared to other functional moieties.[1,2] For the graphene nanopore, the benzenesulfonic functionality dynamically acts as a proton trap and proton shuttle by establishing a favourable confined hydrogen-bond network, resulting in an effective proton channel.[1] In the pristine graphene case, the benzenesulfonic covalent functionality guides the proton hopping toward a distorted basal plane, enabling successive proton tunnelling to the other side of the graphene monolayer.[2,3,4] Notably, in these systems, we achieve estimated proton diffusion coefficients comparable to or higher than the current state-of-the-art PEM with only Nafion.[1,2] The mechanisms exhibited by these benzenesulfonic functionalized graphene-based systems set the ground for designing new 2D-PEMs with efficient unidirectional proton transport features.

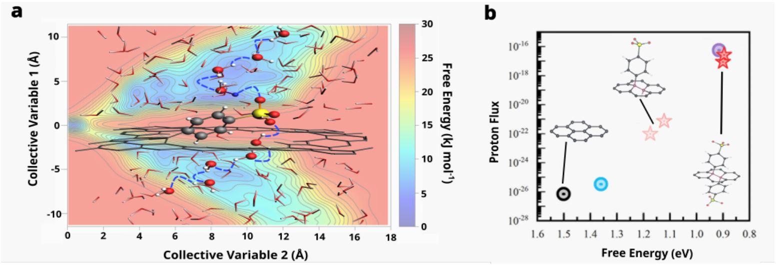

Figure 1. ***a,*** *Free energy profiles (kJ mol^{-1}) along two collective variables (Å) from ReaxFF-MD metadynamics simulations for a graphene nanopore functionalized with benzenesulfonic groups.* ***b,*** *Transmembrane transport proton flux with different benzenesulfonic functionalized pristine graphene monolayers vs corresponding DFT free energy barriers (eV). The flux was simulated using the*

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Wed 12:00–12:30: Invited Talk – Thomas Kühne

Quantum Mechanics in a Glass of Water

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Even at ambient conditions, liquid water can be viewed as a mild quantum fluid. Combining path-integral molecular dynamics with the second-generation Car-Parrinello method, these nuclear quantum effects can be studied together with the quantum mechanical nature of hydrogen-bonding. The effectiveness of this new combined approach is demonstrated on liquid water, ice and the water/air interface with a particular emphasis on on-water catalysis.

Wed 13:30–14:00: Invited Talk – Thomas Heine

Thermodynamic limits of chemical affinity sieving

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Chemical affinity sieving exploits the zero-point energy differences of light-weight atoms or molecules strongly adsorbed at active sites, which typically are undercoordinated metal atoms. Such sites are found in some metal-organic frameworks and in zeolites, where they are typically located in or next to a cavity. We show that the cavity strongly contributes to the thermochemical properties of adsorbed dihydrogen isotopologues and helium isotopes.

We formulate a numerical model of the adsorption sites and demonstrate how the interplay of cavity and metal site controls the thermodynamics to the point that very high selectivities are possible.

Further, we study the adsorption of helium isotopes on gas phase clusters and find surprisingly high adsorption energies, allowing for ^{3}He/^{4}He sieving at 77K. Based on the small clusters, we investigate exemplary materials, i.e. crown ethers, zeolites and MOFs, with similar adsorption sites. While the materials systems show lower selectivity compared to the gas phase clusters, they still are found to be suitable for ^{3}He/^{4}He separation at 20K and, with lower selectivity, at 77K.

Wed 14:00–14:15: Contributed Talk – Felix Moncada

Nuclear orbitals within the Born-Oppenheimer approximation

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Over the past two decades, multicomponent methodologies based on orbitals (single-particle wavefunctions) have emerged as promising approaches to include nuclear quantum effects (NQEs) in molecular and materials simulations[1]. Such calculations directly capture NQEs like zero-point energies and anharmonicity at costs comparable to standard electronic Hartree-Fock (HF) or DFT single-point calculations. However, a key challenge for these multicomponent nuclear orbital methodologies is describing nuclear–electron correlation effects. To avoid these complications, in this work we describe the nuclear wavefunction as a product of orbitals with a Hamiltonian that contains the Born-Oppenheimer potential energy surface.

As a first application, we analyzed the nuclear spin effects of two ^3He atoms encapsulated in C_{60}[2]. At the HF level, the nuclear orbital wavefunction breaks the spin and spatial symmetries, as localized nuclear orbitals have lower energy relative to delocalized, symmetry-adapted ones. To restore the symmetry, we employed a non-orthogonal configuration interaction (NOCI) approach, mixing the broken-symmetry states. The ^3He NOCI states are delocalized, consistent with the near-free rotation of a He_2 pseudomolecule, and they exhibit a splitting pattern that reflects the icosahedral symmetry of the fullerene (Figure 1).

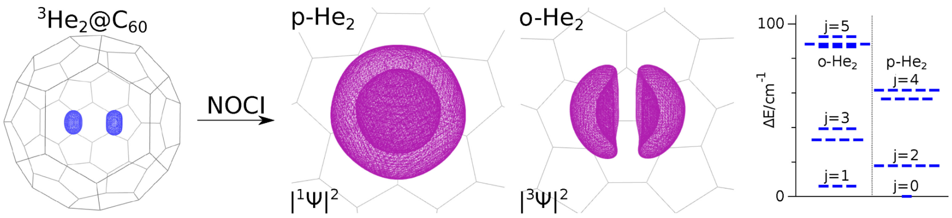

Figure 1. Localized and delocalized nuclear densities and energies of a He_2 pseudo-molecule with nearly free rotation inside the C_{60} icosahedral potential

We have also applied the nuclear-orbital NOCI to analyze NQEs in short, strong hydrogen-bonded systems. The NOCI zero-point and vibrational excitation energies computed are in excellent agreement (within 1 cm^{-1}) with grid-based numerical solutions of the 3D Schrödinger equation for the bonding hydrogen. We are now applying the nuclear-orbital NOCI approach to investigate H^+/D^+ transport through graphene, seeking correlations between the overlap of nuclear states and the corresponding tunneling splitting and tunneling rates.

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Wed 14:15–14:30: Contributed Talk – Daniela Mondonico

Design principles for isotopologue-selective membranes in aqueous environment: the interplay between pore size and functional group chemistry

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The separation of hydrogen isotopes (H, D, and T) represents a critical bottleneck for next-generation nuclear fusion energy and heavy water production. Traditional separation methods remain energetically prohibitive due to the subtle physicochemical differences between isotopologues. This work investigates the exploitation of Nuclear Quantum Effects (NQEs) in functionalized Covalent Organic Framework (COF) membranes to achieve isotope-selective water transport under ambient conditions.

Using Reactive Molecular Dynamics (ReaxFF) simulations, we established a mechanistic framework for H_2O/D_2O discrimination. The central hypothesis posits that isotope-dependent hydrogen bonding between confined water molecules and COF pore walls can be engineered to induce selective transport. While H_2O and D_2O are nearly indistinguishable classically, hydrogen bonds involving the heavier isotopologue are intrinsically stronger due to lower zero-point energy (ZPE).

Our results demonstrate that selectivity emerges as a synergistic product of pore geometry and functional group chemistry. We identified a sub-nanoscale confinement regime where bidentate carboxylic acid groups function as "crossing assistants," facilitating D_2O transport through a dynamic coordination mechanism. Conversely, our analysis of alternative functionalizations reveals that excessively rigid or isolated sites can act as kinetic traps, hindering rather than assisting transport.

This thesis derives rational design principles for isotopic separation, highlighting that optimal membrane performance requires a delicate balance between high binding affinity and dynamic exchange flexibility. These findings provide a roadmap for the development of isotope-selective COF membranes, moving beyond classical separation limits.

Wed 14:30–15:00: Invited Talk – Hoi Ri Moon

Metal–Organic Frameworks as Quantum Sieving Platforms for Next-Generation Hydrogen Isotope Separation

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Efficient separation of hydrogen isotopes remains a central challenge for fusion energy, isotope labeling, and quantum technologies, largely due to the nearly identical physicochemical properties of H_2, D_2, and T_2. Conventional strategies rely on cryogenic distillation with extremely low selectivity, underscoring the urgent need for solid-state alternatives.[1,2] Here, we present a comprehensive exploration of quantum-sieving–based separation using a diverse platform of metal–organic frameworks (MOFs) that collectively demonstrate new thermodynamic, kinetic, and dynamic approaches to isotope discrimination. We first establish that introducing locally flexible diffusion barriers into isoreticular IRMOFs enables kinetic quantum sieving (KQS) at elevated temperatures up to 100 K, achieving ~1.0 mmol g^{-1} D_2 uptake through temperature-dependent aperture modulation.[3] Complementarily, Hofmann-type MOFs with exceptionally dense open metal sites exhibit strong chemical affinity quantum sieving (CAQS), giving a selectivity of 21.7 and D_2 uptake of 10 mmol g^{-1} at 25 K.[4] Building on this, a hybrid CAQS–KQS design in imidazole-functionalized MOF-74 achieves a record separation factor of ~26 at 77 K.[5] Beyond static frameworks, we demonstrate that the breathing transitions of MIL-53(Al) provide dynamic, tunable apertures capable of D_2-selective adsorption, including an unprecedented isotope-responsive *secondary breathing* transition observed exclusively for D_2 by in situ neutron diffraction.[6] Finally, temperature-programmed desorption studies of H, D, and T in MOF-74 reveal systematic isotope-dependent binding and competition, offering quantitative insights relevant to fusion-fuel handling. Together, these studies establish MOFs as a versatile, energy-efficient platform for next-generation hydrogen-isotope separation.

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[2] Jin Yeong Kim, Hyunchul Oh,* and Hoi Ri Moon*, *Adv. Mater.,* **2019**, *31*, 1805293.
[3] Jin Yeong Kim, Linda Zhang, Rafael Balderas-Xicohtencatl, Jaewoo Park, Michael Hirscher*, Hoi Ri Moon*, and Hyunchul Oh*, *J. Am. Chem. Soc.*, **2017**, *139*, 17743.
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Posters

P01: Felix-Florian Delatowski

A Digital Microfluidics Platform for Micro-Batch Processing of Deuterated Species and Photocatalytic Reactions

Felix-Florian Delatowski[a], Julian Appel[b], Anish Das[a], Kirsten Zeitler[b] and Detlev Belder[a]

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Miniaturization and automatization are key components for fast parameter screening and efficient optimization of reaction conditions, paving the way for closed-loop chemistry and the integration of machine learning.[1] Therefore, lab-on-a-chip approaches can yield a convenient “all-in-one” solution, capable of handling tasks such as reactant mixing, real-time monitoring of reaction parameters, performing separation processes, and enabling sensitive analyte detection and quantification.[2] Here, digital microfluidics (DMF) provides a promising technique for discrete droplet handling in an automated and flexible manner and especially its coupling with optical spectroscopy enables real-time, label-free, non-invasive and highly sensitive detection in microscale chemistry.[3]

In this work, a digital microfluidics chip for automated actuation of single droplets, based on the principle of “electrowetting on dielectric”, is presented. To provide a platform for optical analytics, the DMF-chip was optimized for high transparency across the visible and near UV-range. Therefore, the fully transparent design of the top and bottom plates enables a wide range of detection methods, such as UV/Vis, Raman, and surface enhanced Raman spectroscopy (SERS), and allows for efficient on-chip photocatalytic reactions.[4]

As an application, deuteration reactions of organic compounds, such as anisole and diethyl malonate, were selected, and comprehensive off-chip studies and spectroscopic characterization were performed. Finally, initial Raman measurements conducted directly on the DMF chip are presented as preliminary on-chip results.

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P02: Masoud Sadeghi

Experimental Framework for Tritium Breeding Studies in Advanced Ceramic Breeder Materials

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Hydrogen is the most abundant element in the universe, and its heavy isotopes (^{2}H, deuterium, and ^{3}H, tritium) serve as the primary fuels for fusion reactors. While deuterium is readily available on Earth, tritium is extremely scarce and unstable, necessitating its artificial production (breeding) to ensure sustainable reactor operation.

Several tritium-breeding concepts have been proposed, including biphasic Advanced Ceramic Breeders (ACBs) composed of pebbles made from lithium orthosilicate (Li_4SiO_4) and lithium metatitanate (Li_2TiO_3) (Fusion Eng. Des). [1] These ceramic materials exhibit enhanced mechanical performance and possess high lithium content, making them strong candidates for deployment in fusion blanket systems for tritium generation.

Recently, we reported the experimental setup and preliminary analyses related to the initial assessment of tritium breeding in Advanced Ceramic Breeder (ACB) systems (ECCE&ECAB2025). [2] In this work, we present an experimental framework for investigating hydrogen absorption in ceramic breeder pebbles. Potential extensions and improvements to the current experimental design are also discussed.

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P03: Yamini Nirwan

Electrochemical Hydrogen–Deuterium Isotope Exchange in Amines

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Deuterium labelling is a key strategy in mechanistic studies, bioanalysis, and pharmaceutical research. Selective hydrogen–deuterium (H/D) substitution can improve metabolic stability and pharmacokinetic properties due to the kinetic isotope effect. The clinical approval of **Deutetrabenazine** highlights the increasing importance of efficient and selective deuteration methods.[1]

Conventional H/D exchange often relies on transition-metal catalysis or harsh conditions, limiting functional group tolerance and late-stage applicability.[2] Electrochemical synthesis offers a sustainable alternative, enabling redox activation under mild conditions without stoichiometric oxidants.[3] While electrochemical C–H functionalization has advanced significantly,[4] selective electrochemical H/D exchange in amines remains underexplored.

This project aims to develop a metal-free electrochemical hydrogen isotope exchange platform enabled by cooperative supramolecular D-bonding assemblies. Fluorinated alcohols such as HFIP can stabilize reactive intermediates through hydrogen-bonding networks,[5] potentially enabling controlled C–H activation and deuterium incorporation from sustainable sources (e.g., D_2O). This strategy has been successfully translated to hydrogen isotope exchange chemistry, where a cooperative HFIP–water–anion assembly was shown to promote selective deuterium incorporation into aromatic compounds.[6] By integrating supramolecular solvent effects with electrochemical activation, this work seeks to establish a broadly applicable and environmentally benign strategy for late-stage deuteration of amines. Herein, we present the recent results from our ongoing project on electrochemical deuteration at the α-position of cyclic amines.

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[6] Ni, Y.; Lebelt, J.; Barp, M.; Kreuter, F.; Buttkus, H.; Jin, J.; Kretzschmar, M.; Tonner-Zech, R.; Asmis, K. R.; Gulder, T. *Angew. Chem. Int. Ed.* **2025**, *64* (6).

P04: Hyunlim Kim

Carbon Molecular Sieves with Thermally Tunable Pores Enable High-Temperature Quantum Sieving of Hydrogen Isotopes

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Separating hydrogen isotopes is vital for nuclear fusion and diverse industrial applications, yet remains challenging due to their nearly identical physicochemical properties. Kinetic quantum sieving (KQS) offers a promising solution by exploiting subtle differences in diffusion within ultramicroporous environments. While metal–organic frameworks (MOFs) exhibit high selectivity through tunable pores, practical use is often hindered by high costs and limited stability. In contrast, carbon-based materials offer robustness and scalability, but their typically amorphous nature has limited effective KQS, especially at elevated temperatures.

Here, a carbon molecular sieve (CMS) membrane with a bottleneck pore architecture is demonstrated to enable selective hydrogen isotope separation at elevated temperatures. The constricted pore apertures restrict hydrogen diffusion at low temperatures, while thermally induced expansion above 77 K promotes preferential adsorption of heavier isotopes. Temperature-dependent aperture modulation preserves isotope selectivity even above 111 K, a range compatible with existing liquefied natural gas (LNG) infrastructure. These results highlight a scalable and economically viable pathway toward energy-efficient hydrogen isotope separation, connecting advances in porous carbon design with practical prospects for industrial implementation.

P05: Prantik Sarkar

Exploring the potential of CALF-20 for H_2/D_2 separation: Relation between textural properties and isotope separation behavior

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Calgary Framework 20 (CALF-20) is a zinc-based MOF known for its ultra-microporous structure, high stability and excellent gas-adsorption performance. It has been extensively studied for CO_2 capture, showing high selectivity over N_2 and good performance under humid conditions (1).

In this work, we have characterized CALF-20 with advanced physisorption techniques and investigated its hydrogen isotope separation performance using Thermal Desorption Spectroscopy technique. Although several studies have highlighted its selective CO_2 capture and separation performance, a comprehensive characterization of pore network using different adsorbates remains lacking. Given its ultra-microporous structure, we have conducted CO_2 adsorption measurements at 273 K, complemented by dedicated NLDFT kernel, to evaluate its pore size distribution. However, limitations in fully detecting the entire pore size distribution at 273 K require the adoption of an alternative measurement method. We propose a novel characterization technique employing CO_2 adsorption at 220 K, (close to the triple point of CO_2) to achieve a comprehensive textural characterization for the first time.

Low temperature H_2 and D_2 isotherms exhibited multiple step adsorption behavior followed by nearly zero hysteresis. This indicates sequential adsorption in pores where smaller pores get filled at relatively lower pressure region. Higher affinity of the framework towards D_2 was further indicated by the appearance of D_2 sorption steps at a lower pressure than that for H_2.

Isotope separation performance was evaluated using an equimolar mixture of H_2 and D_2. The observed rise in selectivity at T_{exp} = 30K from 3 to 11 as the gas mixture pressure increases from 10 mbar to 100 mbar could be explained from pure gas isotherms. These collective advancements underscore the potential of CALF-20 as a next generation adsorbent for efficient hydrogen isotope separation.

[1] Jian-Bin Lin *et al., Science* ***2021*****,** *374,1464-1469*

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P06: Jaewoo Park

Isotope-Dependent Pore Condensation in the Mesoporous MOF (PCN-222)

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Hydrogen isotope separation in porous materials has been studied predominantly through quantum sieving in microporous systems (Eur. J. Inorg. Chem.).[1] However, condensation in confined pores may also provide a distinct separation mechanism, because the relative pressures for pore filling can differ between isotopes. Here, we show that the mesoporous MOF PCN-222 (ACS Appl. Mater. Interfaces.),[2] featuring well-defined ~31 Å channels and high structural stability, serves as a useful platform to investigate this possibility.

High-resolution adsorption isotherms of H_2 and D_2 reveal a clear difference in the filling pressures of the two isotopes in PCN-222, indicating isotope-dependent condensation behavior within the mesopores. These results suggest that confined condensation, beyond conventional quantum sieving, can be exploited for hydrogen isotope separation.

To probe the confined phase at the microscopic level, we performed in-situ neutron scattering on H_2-, D_2-, and mixed-gas-loaded samples. Although the neutron data show pressure-dependent changes after gas loading, definitive structural assignment remains challenging because of strong incoherent scattering from hydrogen and overlapping framework/gas contributions. Therefore, the neutron results are interpreted as complementary qualitative evidence.

Overall, this work highlights confinement-induced condensation as a promising and previously underexplored route for hydrogen isotope separation and establishes PCN-222 as a robust model system for studying isotope-dependent phase behavior in mesoporous frameworks.

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P07: Zheng Li

Fit4H2: Optoelectronic strategies for hydrogen detection in industrial application

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In recent years, with the growing concern over global warming and climate change, hydrogen has attracted increasing attention as a clean energy carrier in renewable energy systems. As the hydrogen market continues to expand, the demand for hydrogen transportation is also increasing. Whether hydrogen is transported in cylinders, tanks, or pipelines, reliable hydrogen leakage detection is essential for ensuring operational safety.

In addition, hydrogen, being the lightest gas, can easily permeate into many metallic materials. Hydrogen permeation may lead to hydrogen embrittlement, which can cause material degradation and eventually result in leakage or structural failure. Therefore, besides conventional hydrogen leakage monitoring, the detection of hydrogen at extremely low concentrations can also serve as an effective indicator for hydrogen permeation and potential embrittlement within materials. In this case, ultra-high resolution of hydrogen detection is developed in demand.

In this project, aiming at industrial hydrogen detection applications, an experimental setup was developed for hydrogen sensing measurements. Optical sensing measurement was conducted and optoelectronic sensing strategies were explored. Patterned samples were fabricated using electron beam lithography. The interaction between hydrogen and the sensing materials was indicated by wavelength shifts in the optical signal. Future work will focus on exploring additional sensing materials and pattern designs to further improve sensing performance.

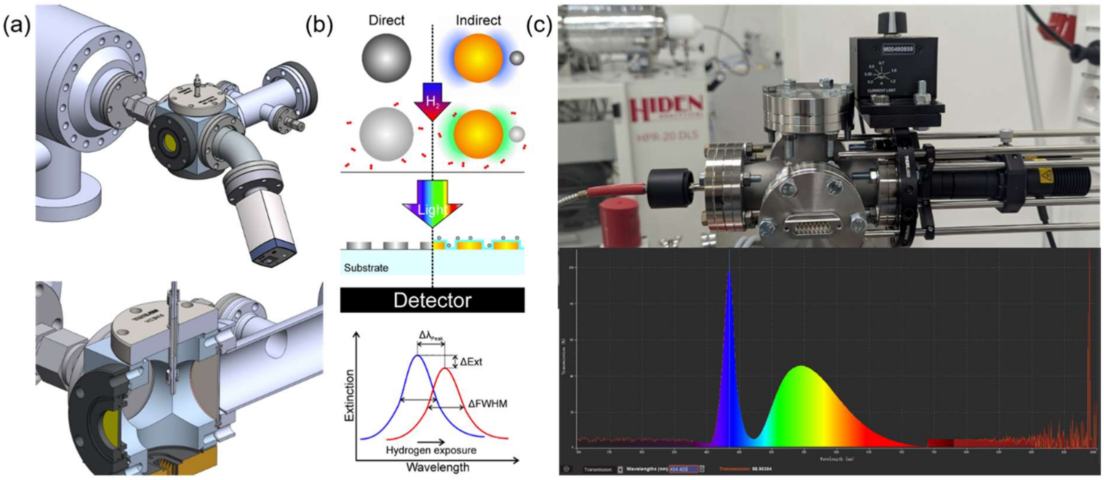

Figure 1: (a) Measurement setup (b) Wavelength shift indicated the interaction between materials and hydrogen (c) conducted setup and measured wavelength under different light source

P08: Jing Liu

Tritium, deuterium, protium separation using Ni-MOF-74 investigated by thermal desorption spectroscopy

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Deuterium (D) and tritium (T) are heavy isotopes of protium (H) that play essential roles in isotope labeling, environmental tracing, and nuclear fusion. Developing efficient strategies for hydrogen isotope separation is therefore of great importance for both scientific and technological applications. Ni-MOF-74 has previously been reported to show promising selectivity for H/D separation[1], attributed to its open metal sites and well-defined channels. Here, we extend this concept by systematically investigating the adsorption-desorption behavior of all hydrogen isotopes, including tritium. We quantified the separation using thermal desorption spectroscopy (TDS), monitoring the desorption of isotopes with mass spectrometry during heating from 82 K to 300 K. The setup included a CuO flow reactor to convert the desorbed T_2 to HTO, which was analyzed by liquid scintillation counting to calibrate the MS signal for tritium.

Temperature-controlled desorption of the pure isotopologues indicates progressively stronger binding for the heavier isotopes. In binary and ternary mixtures, differences in adsorption affinity lead to competitive adsorption, such that heavier isotopes preferentially occupy the binding sites, resulting in strongly temperature-dependent selectivity. Specifically, binary mixtures at 82 K exhibited a T_2/H_2 separation factor of 10.9. In an initially equimolar (1:1:1) ternary mixture, the tritium fraction rose to 55.3% at 82 K and to 79.5% when the exposure temperature was raised to 101 K. These results confirm the strong isotope-dependent affinity to open metal sites of Ni-MOF-74, demonstrating its efficiency for separating gaseous hydrogen isotope mixture at mild cryogenic temperatures above 77 K.

[1] J. Y. Kim, R. Balderas-Xicohténcatl, L. Zhang, S. G. Kang, M. Hirscher, H. Oh and H. R. Moon, *Journal of the American Chemical Society* **2017**, *139*, 15135-15141.

P10: Rhyan Barrett

Incorporating long interactions into machine learning potentials via the multipole expansion

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Simulating long-range interactions remains challenging for molecular ML potential because interactions must be captured across large spatial regions. Here we integrate a multipole expansion into equivariant ML potentials to model long-range effects in QM/MM simulations for both ground and excited states. Benchmarks show improved prediction of energies and forces for nickel complexes and enable simulation of excited-state dynamics in solutions. Transfer learning from foundational models further improves data efficiency, reducing the need for large QM/MM datasets.

P11: Hannah Buttkus

Hydrogen Isotope Effects Used to Reveal Vibrational Signatures of a Microsolvated Hexafluorophosphate Anion

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Hexafluorophosphate (PF_6^-), widely used in lithium-ion batteries and known to release biologically damaging hydrofluoric acid upon hydrolysis, has recently been detected in environmental waters.[1,2] Molecular-level insight into its interactions with solvents like water or 1,1,1,3,3-hexafluoroisopropnaol (HFIP), which catalyze PF_6^- hydrolysis, is therefore crucial for understanding solvation behaviour and for providing reliable input to computational simulations.[2]

In this ongoing study, we investigate how HFIP and its isotopologues influence the microhydration of PF_6^-. The complexes $PF_6^-(HFIP)_x(H_2O)_y$ are systematically investigated by IR photodissociation spectroscopy in the spectral region between 800 – 4000 cm^{-1} and assigned using electronic structure calculations.

In single-solvent complexes, HFIP and H_2O each engage in weak hydrogen bonding with PF_6^-, as indicated by O-H stretching frequency shifts $\Delta\nu(\mathrm{OH})$ of less than 200 cm^{-1}. Additional HFIP molecules continue to engage in ionic hydrogen bonding, while H_2O molecules prefer to form an intramolecular hydrogen-bonded network on one side of the anion, whereas HFIP primarily engages in ionic hydrogen bonding. In mixed-solvent $PF_6^-(HFIP)(H_2O)_x$ (x = 1-5) complexes, HFIP is incorporated into the hydrogen-bonded network, cooperatively strengthening the inter-solvent hydrogen bond ($\Delta\nu(\mathrm{OH})$ = 873 cm^{-1}) while weakening the PF_6^- - water interaction ($\Delta\nu(\mathrm{OH})$ = 91 cm^{-1}). In $PF_6^-(HFIP)_x(H_2O)$ (x = 1-3) complexes, additional HFIP molecules weaken the HFIP - water hydrogen bond yet simultaneously promote solvation-enhanced proton transfer between PF_6^- and water, offering first molecular evidence for the onset of HFIP-catalyzed PF_6^- hydrolysis.

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P12: Minji Jung

Investigation of Adsorption Mechanisms in Metal-Organic Frameworks for Hydrogen Isotope Separation

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Nuclear fusion has been considered as promising and clean energy source, and is capable of solving the anticipated energy crisis. Deuterium (D_2) is a fuel for the nuclear fusion process which makes it crucial considering the demand for clean energy in the future. However, its natural abundance is quite low and its separation from hydrogen isotope mixture is also challenging due to its identical size, shape and thermodynamic properties. Currently, D_2 can be separated either by using the Gridler-sulfide process(GS) or Cryogenic distillation, but these two methods entail low separation efficiencies and high energy consumption. Hence, it necessitates the development of the more efficient separation technology. Recently, D_2 separation from hydrogen isotope mixture using crystalline nanoporous materials through the quantum sieving effect has been launched as a promising and cost-effective approach. We reported previously an additional adsorption phenomenon that occurs exclusively with D_2, attributed to its dense packing compared to H_2, in the cobalt formate (CoFA), a type of Metal-Organic Framework. (MOFs) [1] To understand this unique behavior, a detailed analysis of the adsorption mechanisms of both H_2 and D_2 within CoFA is essential.

Herein, in-situ neutron powder diffraction (NPD) measurements were performed to investigate the adsorption behavior of hydrogen isotopes within the CoFA framework. Hydrogen isotopes were introduced into the pores with controlled loading amounts, and NPD patterns were collected at each loading step. The obtained diffraction patterns were analyzed by Rietveld refinement, enabling identification of the adsorption sites of hydrogen isotopes within the framework. By tracking the evolution of the diffraction patterns as a function of loading, the adsorption configuration of hydrogen isotopes was examined. This structural analysis provides direct insight into the adsorption sites responsible for isotope uptake and helps clarify the adsorption mechanism governing hydrogen isotope separation in CoFA.

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P13: Julian A. Thoma

Tritium Labeling Strategies for different Pyrethroid Pesticides

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Pyrethroids are a class of synthetic insecticides chemically modeled after natural pyrethrins found in chrysanthemum flowers. Since their commercial introduction in the 1970s, they have become one of the most widely used pesticide groups globally, replacing more acutely toxic organophosphates in the agricultural sector. To accurately investigate the metabolic fate and environmental distribution of these compounds, Tritium radiolabeling is an essential tool. However, the complex molecular architecture of pyrethroids, characterized by multiple chiral centers and reducible functional groups, presents significant challenges for traditional Tritium chemistry [1, 2].

This study evaluates and optimizes diverse labeling strategies and reaction conditions to produce highly pure radioligands with good specific activities. By employing Tritium-NMR spectroscopy, we precisely determined the sites of isotopic insertion, providing critical insights into the underlying reaction mechanisms and establishing a robust methodology for developing tracers suitable for toxicological and environmental research.

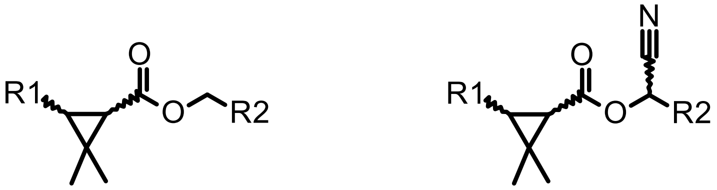

Figure 1: Type I Pyrethroid insecticide (left), Type II Pyrethroid insecticide (right).

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P14: Sieeun Jeong

Quantitative Calibration of H2, D2, and HD in TDS for RT Hydrogen Isotope Separation Studies

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Accurate quantification of hydrogen isotopes released from sorbent and hydride-forming materials is essential for evaluating isotope-selective adsorption and separation behavior. In particular, while H2 and D2 are commonly considered in isotope sorption studies, reliable analysis of HD is equally important because mixed-isotope compositions are frequently generated during isotope exchange, sorption-desorption cycling, and practical separation processes. For this reason, an analytical method capable of quantitatively distinguishing and calibrating H2, D2, and HD is required for rigorous assessment of hydrogen isotope separation performance.

Here, we established a quantitative HTDS calibration method including HD using standard materials such as Pd-Ce alloys and TiH2. The calibration enabled reliable isotope analysis over a wide desorption temperature range (RT to 1000C). Using this method, we investigated the room-temperature hydrogen isotope sorption and separation behavior of Pd98Ce2, which exhibits isotope-dependent hydrogen uptake above ambient temperature. Quantitative analysis of desorbed H2, D2, and HD provided direct evidence of isotope-selective behavior under near-practical operating conditions.

The present work highlights the importance of HD-resolved calibration in HTDS analysis and demonstrates its utility for quantitatively assessing hydrogen isotope separation performance in adsorption-based systems.

P15: Jantje P. Bäcker

Acoustofluidic Emulsification – Towards Sensitive ^{3}H-Analysis

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Tritium (^{3}H) is a low-energy β^--emitter that can be well-detected using liquid scintillation counting (LSC). To do so the tritiated sample is mixed with an organic scintillation cocktail. However, if aqueous samples are to be measured the cocktail contains great amounts of surfactants, which account for quenching effects lowering sensitivity (National Diagnostics).[1] This experimental work aims at developing a miniaturized lab-on-a-chip device leading to fast and efficient emulsification while at the same time reducing surfactant concentrations.

Since breaking up two phases is difficult to accomplish in the laminar regime present in most microfluidic devices, adding extra energy is inevitable for bulk emulsification. An efficient way of doing so is attaching a transducer and generating acoustic waves propagating through the system (acoustofluidics) leading to acoustic streaming (figure 1). Therefore, monolithic fused silica chips integrating free-standing cone-shaped rods and a piezo element were manufactured by selective laser-induced etching (SLE), and emulsification tests were performed.

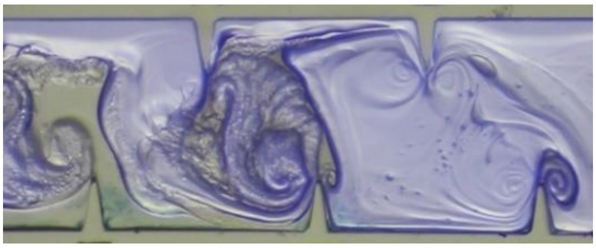

Figure 1: Exemplary fluorescence microscopic image of emulsification process of water and LSC-cocktail due to acoustic streaming in a PDMS-based microfluidic chip.

For a comparison, emulsions were prepared using the conventional method of pipetting the liquids and shaking by hand. All emulsions were analyzed by dynamic light scattering (DLS) measurements giving insight on the size distributions of the water droplets created in LSC-cocktail during emulsification. It was shown that acoustofluidics enable emulsion formation in microfluidic chips including water and LSC-cocktail even with reduced surfactant concentration. This paves the path for sensitive tritium analysis in the future.

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P16: Mahnaz Bakhtian

Bimetallic MOF-74: Fabrication and Comparative Study of H_2/D_2 Uptake

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Hydrogen isotope separation, particularly between protium (H_2) and deuterium (D_2), plays a critical role in analytical, and energy technologies. Yet, the separation remains technically demanding due to the nearly identical size and chemical properties of the isotopologues. Current industrial methods are energy-intensive and often inefficient, underscoring the need for advanced materials that can achieve high selectivity through alternative mechanisms. [1]

Metal–organic frameworks (MOFs) have emerged as promising candidates for this challenge, offering unparalleled tunability in structure and functionality. This project focuses on exploring how tailored modifications to MOFs and their pore properties can enhance their capacity for isotope separation. [2]

In this work, bimetallic MOF-74 frameworks containing Ni–Mn and Ni–Zn were synthesized via a room-temperature method. The obtained materials were characterized by using SEM, EDX, ICP-OES, PXRD, and IR spectroscopy to confirm morphology, composition, and structural integrity. Nitrogen adsorption measurements were conducted to determine surface area and pore size distribution, revealing ultramicroporous structures in both materials. Despite similar pore size distributions, Ni–Zn-MOF-74 exhibited higher BET surface area and enhanced gas adsorption compared to Ni–Mn-MOF-74. Hydrogen (H_2) and deuterium (D_2) adsorption measurements at 77 K and 97 K further demonstrated superior uptake in Ni–Zn-MOF-74. These results indicate that metal composition significantly influences adsorption performance even when pore size characteristics remain similar. Future work will focus on thermal desorption spectroscopy (TDS) to further investigate adsorption behavior and isotope interactions within these frameworks.

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P17: Luis Antonio Panes-Ruiz

Fit4H2: Constructive-technological development and implementation of processes for hydrogen non-permeable pipe and connection systems

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In recent years, hydrogen has attracted significant attention as a low-carbon energy source due to its clean, renewable, and efficient nature. However, ensuring safe production, compression, storage, and particularly transport for use in urban or industrial applications remains a critical challenge. In this context, the project Fit4H2 brings together a German-Italian consortium comprising academic and industrial partners to address the constructive and technological development of processes for coating pipes and fitting connections with defect-free hydrogen barrier layers. These coatings are based on hexagonal boron nitride (h-BN) and metal oxides, such as Al_2O_3 and Al_2O_3:Cr_2O_3, to achieve minimal hydrogen permeability for a wide range of working pressures and temperatures. In addition, the project also targets the development of nanomaterial-based H_2 gas sensors for long-term monitoring with high sensitivity and selectivity.

In this work, we present a theoretical and experimental approach for the study of H_2 gas permeability. On the one hand, the flux calculation based on the diffusion coefficient and the solubility of H_2 in the material, namely copper, stainless steel V4A, and h-BN (Fig.1a). On the other hand, the experimental setup for the quantification of permeated H_2 gas through coated and uncoated stainless steel (V2A & V4A) and cast-iron samples. The system utilizes an ultra-high resolution quadrupole mass spectrometer (QMS), enabling precise detection of permeated gas species. The high resolution of the instrument allows reliable specific peak-separation of D_2^+ in $^4He^+$, while maintaining detection sensitivity in the part-per-billion (ppb) concentration range (Fig 1b). Moreover, we propose an industrially safe plasmonic sensing platform based on palladium nanodot arrays fabricated via electron beam lithography, enabling sensitive optical detection of hydrogen.

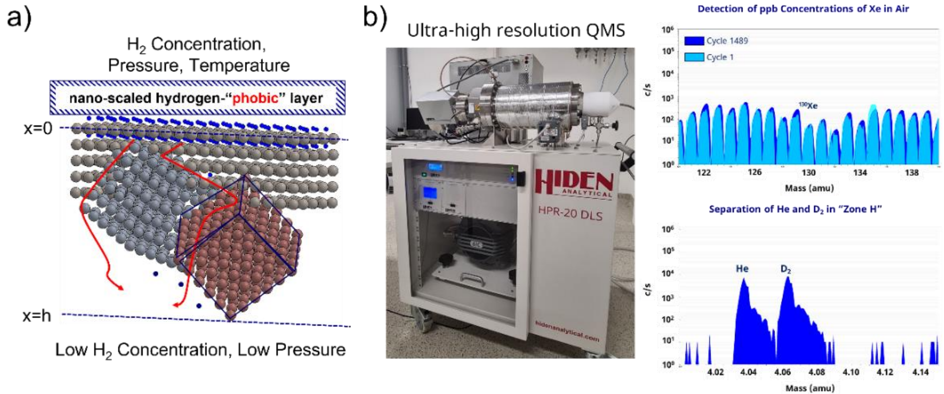

Figure 1: Theoretical (a) and experimental (b) approach for the study of H_2 gas permeability and the development of H_2 barrier coatings.

P18: Sanjay Lama

Automated Microfluidic Enzyme Screening with Online HPLC-MS

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The efficient use of biocatalysts, such as enzymes, is essential for achieving the goal of integrating eco-friendly chemistry into industrial processes, as they enable highly selective reactions under milder and greener conditions.[1–4] Immobilizing these enzymes into miniaturized continuous reactors, such as microfluidic immobilized enzyme reactors (MIERs), can improve stability while simultaneously reducing the consumption of solvents, reagents, and most importantly, valuable biocatalytic material. However, the operation of such reactors, requires a suitable analytical method capable of continuously monitoring their performance. Online HPLC-MS analysis provides a solution, delivering high-quality qualitative and quantitative information in real time, with precise insights into molecular composition, structure, and concentration of biocatalytic transformations.

We present a novel microfluidic screening platform that combines microreactor technology, multi-reactor integration, and online HPLC-MS analysis in a sequential automated workflow.[1] An automated sample feed facilitates the systematic investigation of different substrates and reaction parameters, while external valve control enables contamination-free switching between individual MIERs. The reaction effluent is subsequently analyzed via an integrated commercial LC-ESI-MS unit. Additionally we evaluated a miniaturized, modular chipLC system that shortened the total separation time to 2 minutes and reduced solvent consumption by over 80%. Together, these features provide a faster, resource-efficient platform for enzymatic reaction screening that minimizes biocatalyst consumption while delivering comprehensive, high-quality HPLC-MS datasets on immobilized enzyme performance under continuous-flow conditions. Beyond biocatalysis, the analytical platform presented here can be readily implemented for the low-consumption screening of most heterogeneous catalysts. Moreover, the information obtained offers a valuable foundation for scaling- or numbering-up continuous processes.

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P19: Siyara Kehelwalathenne

Quantifying Isotope Effects on Chemical Bonding in H_2 Adsorption in Metal Organic Frameworks

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Metal organic frameworks (MOFs) are promising materials for hydrogen storage and isotope separation due to their tunable pore structures and strong adsorption sites at open metal centers (OMCs). One mechanism enabling isotope selectivity is chemical affinity quantum sieving, which arises from differences in zero-point vibrational energies and adsorption enthalpies of hydrogen isotopologues.[1][2] Despite extensive studies, a detailed understanding of how ligand environments and metal substitutions modulate the interaction between H_2 and OMCs remains limited.[3]

In this work, density functional theory (DFT) calculations at the B3LYP-D4/def2-TZVPP level were used to investigate how ligand donor environments influence H_2 adsorption at Cu-based metal sites. Fragment models with different numbers of oxygen donor ligands were studied to evaluate their effect on the Cu–H_2 interaction. The adsorption energy of the first H_2 molecule is -28 kJ mol^{-1} for the two-Cu system and -12 kJ mol^{-1} for the three-Cu system. Red shifts of approximately 170 cm^{-1} and 58 cm^{-1} in the H–H stretching frequency are observed upon adsorption, respectively, consistent with IRPD experimental data.To connect the fragment models with realistic framework environments, the Cu paddle-wheel unit of HKUST-1 containing benzene-1,3,5-tricarboxylate linkers was modeled, including Cu–Cu, Cu–Zn, and Zn–Zn metal substitutions.

Energy decomposition analysis-natural orbitals for chemical valence analysis shows that the interaction is dominated by σ-donation from H_2 to the metal center together with π back-donation. To capture nuclear quantum effects and isotope-dependent interactions, NEO-DFT (Nuclear Electronic Orbital DFT) calculations were performed.[4] The results indicate slightly stronger binding for heavier isotopologues, (D_2,T_2) with the metal sites than H_2.

Overall, this work provides molecular-level insight into the factors governing hydrogen adsorption and isotope effects in MOFs, demonstrating that ligand donor environments, metal composition, and nuclear quantum effects collectively influence H_2 adsorption strength and isotope selectivity. These findings contribute to the rational design of MOF materials for improved hydrogen storage and isotope separation.

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P20: Alexander Feige

Combining genetic algorithms with omits in kinematical refinements of cRED data: pathways towards higher accuracy

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Electron diffraction is an essential technique for determining crystal structures. Yet its accuracy frequently suffers due to dynamical scattering effects, leading to significant deviations in reflection intensities.[1]

To address this challenge, we implemented a genetic optimization algorithm designed to selectively refine subsets of reflection data from continuous electron diffraction datasets,[2] thereby enhancing the accuracy of structure refinement. This flexible algorithm accommodates multiple objectives, which can be either dependent or independent of refinement statistics. We tested our approach on datasets from a staircase-like crystal structure of the zeolite STW and multiple crystals of the inorganic salt KH_2PO_4. Our results demonstrate notable improvements in atomic displacement factors and facilitate precise localization of hydrogen atom positions, even under kinematical refinement conditions. These findings highlight the algorithm's efficacy as a practical method for identifying and excluding dataset regions strongly affected by dynamical scattering, being also applicable to other data collection strategies, such as serial electron diffraction.

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P21: Dennis El Mouzawak

Ion Soft-Landing of Undercoordinated Metal Complexes: Spatial Profiling, Ion Beam Control, and Stabilization

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Ion soft-landing[1–3] enables the controlled deposition of mass-selected ions onto surfaces. Recent advances in electrospray ionization (ESI) coupled deposition instruments now allow the formation of thin functional material layers using complex ions from the gas phase.[4–6] Collision-induced dissociation (CID) in the gas phase can be used to generate undercoordinated metal species. We deposited such ions onto layers on surfaces to create new model systems for DHI separation. Preserving ionic charge during deposition, supported by sequential deposition of cations and weakly coordinating anions, is critical for controlling the chemical reactivity of the deposits.[7]

A systematic investigation of the layers formed by co-deposition of the undercoordinated Ru complex with weakly coordinating anions (WCAs; $[B_{12}Cl_{12}]^{2-}$, $[PF_6]^-$) was conducted, with Reflection–Absorption Infrared Spectroscopy (RAIRS) providing detailed insight into the resulting layer compositions. Deposition of the Ru complex without stabilizing WCAs resulted in less abundant IR signals through degradation of the bipyridine ligand, whereas co-deposition with a WCA effectively suppressed this decomposition. To probe the “chemical availability” of the undercoordinated binding site within the layer, the prepared sample was exposed to CO atmosphere and the bound CO was detected by RAIRS. Stabilization by the WCA significantly enhanced CO adsorption at the metal center, which is apparently protected from undergoing undesired side reactions. Because this stabilization requires efficient ion–ion interaction, precise spatial overlap of the deposited cations and anions is essential. However, this approach revealed challenges because cation and anion beams often show a spatial offset at the surface.

To precisely assess the offset of two deposited types of ions across the surface, spatially resolved X-ray Photoelectron Spectroscopy (XPS) measurements were performed. The introduced methods are part of a currently developed procedure to ensure the best possible overlap of ion beams of sequentially deposited ions on surfaces.

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P22: Maria Chiara Crimella

Deposition of charged microdroplets to quantify charge separation of salts in the ESI process

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Electrospray Ionization (ESI) is a widely used technique developed to transfer charged particles from solution into the gas-phase. We investigate how the charge of molecular salts in microdroplets changes dependent on ESI defining parameters (emitter diameter, ESI voltage, distance between the ESI capillary and the surface, flowrate, type of analyte and solution concentration). To do this we deposit microdroplets/ions onto a gold substrate under different vacuum conditions. We start with an atmospheric deposition of charged microdroplets, followed by a rough vacuum deposition (using an ion funnel chamber) and compare these results with an ion soft-landing (ISL) deposition of mass-selected bare ions under high-vacuum conditions of a mass spectrometer. Depending on the ions nature (atomic/molecular) we use different analytical methods (XPS, IR or NMR) to quantify differences in the ratio of anions to cations within the film generated on the gold substrate.

The results of atmospheric ESI depositions of salt solutions were found to be difficult to reproduce. We learned that the composition of the layers formed by collecting microdroplets emitted from the Taylor cone depends on the distance of the ESI capillary and the surface. Moreover, applied ESI voltage and flow rates of the solution have a major impact on the measured deposition current.

With this approach we try to generate insight into what properties salts must have to generate high ion currents through effective ionization.

P23: Daniela Mondonico

Design principles for isotopologue-selective membranes in aqueous environment: the interplay between pore size and functional group chemistry

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The separation of hydrogen isotopes (H, D, and T) represents a critical bottleneck for next-generation nuclear fusion energy and heavy water production. Traditional separation methods remain energetically prohibitive due to the subtle physicochemical differences between isotopologues. This work investigates the exploitation of Nuclear Quantum Effects (NQEs) in functionalized Covalent Organic Framework (COF) membranes to achieve isotope-selective water transport under ambient conditions.

Using Reactive Molecular Dynamics (ReaxFF) simulations, we established a mechanistic framework for H_2O/D_2O discrimination. The central hypothesis posits that isotope-dependent hydrogen bonding between confined water molecules and COF pore walls can be engineered to induce selective transport. While H_2O and D_2O are nearly indistinguishable classically, hydrogen bonds involving the heavier isotopologue are intrinsically stronger due to lower zero-point energy (ZPE).

Our results demonstrate that selectivity emerges as a synergistic product of pore geometry and functional group chemistry. We identified a sub-nanoscale confinement regime where bidentate carboxylic acid groups function as "crossing assistants," facilitating D_2O transport through a dynamic coordination mechanism. Conversely, our analysis of alternative functionalizations reveals that excessively rigid or isolated sites can act as kinetic traps, hindering rather than assisting transport.

This thesis derives rational design principles for isotopic separation, highlighting that optimal membrane performance requires a delicate balance between high binding affinity and dynamic exchange flexibility. These findings provide a roadmap for the development of isotope-selective COF membranes, moving beyond classical separation limits.