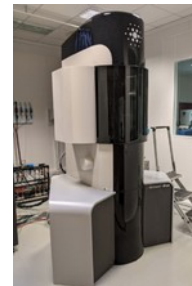# MEM

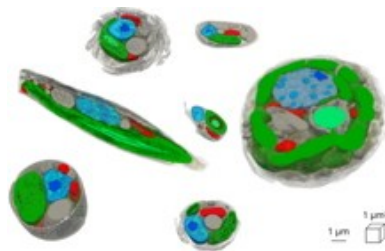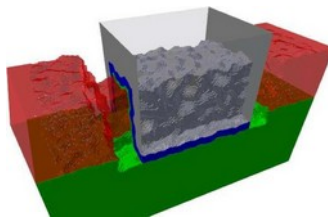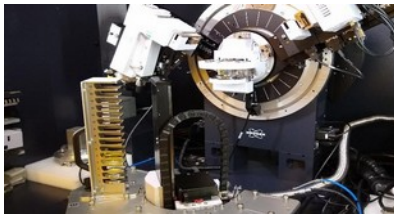## MODÉLISATION, EXPLORATION DES MATÉRIAUX

Materials Exploration and Modelling

Master Thesis Projects

2024

MEM in brief

The MEM laboratory offers a unique and coherent set of techniques for material exploration. It is able to provide comprehensive and concrete answers to materials or processes problems.

The MEM laboratory gathers different teams in our Institute whose thematic area is around one technique or one type of experimental technique.

- **LEMMA team**: Advanced Microscopies laboratory and ion beams. Ultimate TEM, strain measurements, holography, chemical analysis
- **NRX team**: Nanostructures and X-Rays. Studies of nanostructures using laboratory and synchrotron X-rays.
- **NMR team**: Nuclear Magnetic Resonance lab, development of Dynamic Nuclear Polarization/Magic Angle Spinning techniques for solid state NMR.
- **MDN team**: neutron diffraction laboratory. Triple axis inelastic scattering, magnetic scattering. Running of CRG instruments at ILL.
- **L_SIM team**: numerical simulation laboratory, developing and using *ab initi*o codes based on DFT, Tight binding, GW methods etc.

The competencies and experimental tools of MEM laboratories are also an essential part of the Grenoble nano-characterization platform (PFNC) and other collaborating research groups (CRGs) built around Grenoble large facilities (ILL for neutrons and ESRF for synchrotron).

Projet bibliographique - Stage de recherche M2

Solid-state NMR studies of cathode materials for aqueous rechargeable Li-ion batteries

Project description

Li-ion batteries are of tremendous importance in our lives, but can pose serious safety hazards due to the use of highly flammable organic electrolytes – news of battery fires and explosions seem to appear on a regular basis. Replacing the organic electrolyte with a water-based system is an attractive solution to increase battery safety while at the same time reducing cost and environmental impact. However, Li-ion batteries with aqueous electrolytes currently suffer from low energy density and short cycle life. A detailed mechanistic understanding of the underlying reasons for this is often lacking, as most research to date has focused on the well-established organic electrolytes. For example, little attention has been paid to the interaction of Li-ion battery electrode materials – generally used in proton-free environments – with the water in aqueous electrolytes.

The goal of this project is to use solid-state NMR spectroscopy to investigate the behavior of common Li-ion battery positive electrode materials in aqueous electrolytes as a function of battery cycling. It will involve laboratory work on Li-ion batteries (electrode preparation, battery assembly, electrochemical cycling) as well as solid-state NMR measurements of cycled electrodes prepared within the project. This provides the exciting opportunity to acquire skills in two complementary fields: Li-ion batteries and solid-state NMR spectroscopy.

Master student profile and qualifications

This project suits candidates following a master in Chemistry, Physical Chemistry, Materials Science, Electrochemistry or related fields with a strong interest in spectroscopy. Knowledge in NMR and/or Li-ion batteries will be a plus. Excellent communication skills in English and the ability to work in a research team are required.

How to Apply

Interested candidates should send a short motivation letter, a CV, and transcripts of grades (License, M1) to Katharina Märker (katharina.marker@cea.fr).

Scientific environment and workplace

The successful candidate will join the Magnetic Resonance (RM) laboratory at the Interdisciplinary Research Institute of Grenoble (IRIG). The laboratory is composed of five permanent researchers/assistant professors, one research-engineer, one technician, and multiple PhD students and postdocs. It hosts three research-oriented NMR spectrometers (200 / 400 / 500 MHz) equipped with state-of-the-art solution NMR, PFG, HRMAS and solid-state NMR

probes. Furthermore, the laboratory is equipped with advanced solid-state NMR equipment, including two MAS-DNP systems, a home-built sustainable helium sample spinning system for ultra-low temperature MAS NMR and DNP, and an operando NMR setup for battery studies. The originality of the RM lab lies in the diversity of its research, which encompasses method development and major instrumental developments, but also advanced applications in battery research, functional materials, and complex biomolecular systems. RM lab members also have access to the battery research platform at IRIG.

The Magnetic Resonance laboratory is part of the Modeling and Exploration of Materials Laboratory (MEM), a joint research unit of the CEA and the Université Grenoble Alpes. The MEM belongs to the Interdisciplinary Research Institute of Grenoble (IRIG), which gathers 10 laboratories and around 1000 researchers, technicians, doctoral and post-doctoral students, covering a large variety of interdisciplinary fields (nanophysics, chemistry for health and energy, cryo-technologies, biology and medicine). Besides, IRIG includes also the IBS NMR groups, which are specialized in structural biology and host six NMR instruments, including a 950 MHz spectrometer. This strong environment in NMR is ideally complemented by research teams specialized in EPR, advanced electron microscopy, X-ray (lab equipment and ESRF) and neutron diffraction (ILL).

Located in the French Alps and surrounded by a stunning natural environment, the international city of Grenoble represents an extremely rich ecosystem formed by public research organizations (CEA, CNRS, ESRF, ILL) and high-tech companies. In addition, the Université Grenoble Alpes attracts a large number of students who can benefit from high-level academic training in a broad range of disciplines.

More information about the group [here](#), [here](#) and [here](#).
More information about the IRIG institute [here.](#)

References related to the topic
K. Märker, C. Xu, C. P. Grey (2020) Operando NMR of NMC811/Graphite Lithium-Ion Batteries: Structure, Dynamics, and Lithium Metal Deposition. *J. Am. Chem. Soc. 142*(41), 17447–17456.
https://doi.org/10.1021/jacs.0c06727

K. Märker, P. J. Reeves, C. Xu, K. J. Griffith, C. P. Grey (2019) Evolution of Structure and Lithium Dynamics in LiNi$_{0.8}$Mn$_{0.1}$Co$_{0.1}$O$_2$ (NMC811) Cathodes during Electrochemical Cycling. *Chem. Mater. 31*(7), 2545–2554.
https://doi.org/10.1021/acs.chemmater.9b00140

A. Cresce, K. Xu (2021) Aqueous lithium-ion batteries. *Carbon Energy 3*(5), 721–751.
https://doi.org/10.1002/cey2.106

Projet bibliographique - Stage de recherche M2

Operando NMR of Li-ion batteries: Pulse sequence development and optimization

Project description

Li-ion batteries are of tremendous importance in our lives, with the ever-increasing demand for higher energy density and longer lifetimes posing great challenges for research and development. Operando NMR is a powerful technique for studying the working mechanisms and degradation processes in Li-ion batteries. Since these measurements are performed on *working* batteries, they provide invaluable real-time insights, but are also extremely challenging given that battery cycling and NMR spectroscopy have to be combined. Therefore, NMR experiments in operando measurements are usually rather simple and limited to the detection of abundant species in the cell.

The goal of this project is to advance operando NMR of Li-ion batteries through the use of advanced multi-pulse sequences and double-resonance experiments. The student will learn about static solid-state NMR pulse sequences and work on their practical implementation on the spectrometer. Moreover, they will assemble their own batteries in order to test the pulse sequences on ex situ battery samples. Depending on the progress of the project, operando NMR experiments may be performed as well.
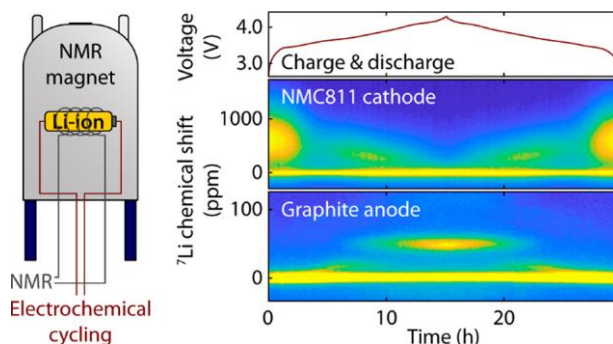
Master student profile and qualifications

This project suits candidates following a master in Chemistry, Physical Chemistry, Materials Science, Physics or related fields with a strong interest in spectroscopy. Knowledge in Li-ion batteries is not required, but will be a plus. Excellent communication skills in English and the ability to work in a research team are required.

How to Apply

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https://doi.org/10.1021/jacs.0c06727

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https://doi.org/10.1021/acs.chemmater.9b00140

Projet bibliographique - Stage de recherche M2

Probing surface chemistry of halogenated perovskite nanocrystals using NMR and Dynamic Nuclear Polarization

Contact subhradip.paul@cea.fr and gael.depaepe@cea.fr

Project description:

The discovery of $CsPbBr_3$ nanocrystals in 2015 and their unique light-emitting properties have generated significant research interest.[1–2] Like for most semiconductor nanocrystals, the ligands are key to control both the growth (size and shape), but also the colloidal stability of halogenated perovskite nanocrystals (PNCs). In addition, the ionic nature of the core (Figure 1a) makes them very different from other covalent semiconductor NCs (CdSe, ZnO, ZnS, etc.), and particularly prone to degradation from factors such as light, humidity, and heat. Understanding the surface chemistry of these systems is thus mandatory to further improve rationally both the reproducibility of hot-injection synthesis (using the so called native ligands), and the colloidal stability through ligand-exchange. Native ligands for $CsPbBr_3$ NCs are typically composed of long chain alkylammonium (e.g. oleylammonium) and carboxylates (e.g. oleate). Recently, several research groups have used theoretical and experimental approaches to study the surface termination of these systems and the role of passivating ligands. This includes the use of both liquid and solid-state NMR approaches.[3–5]
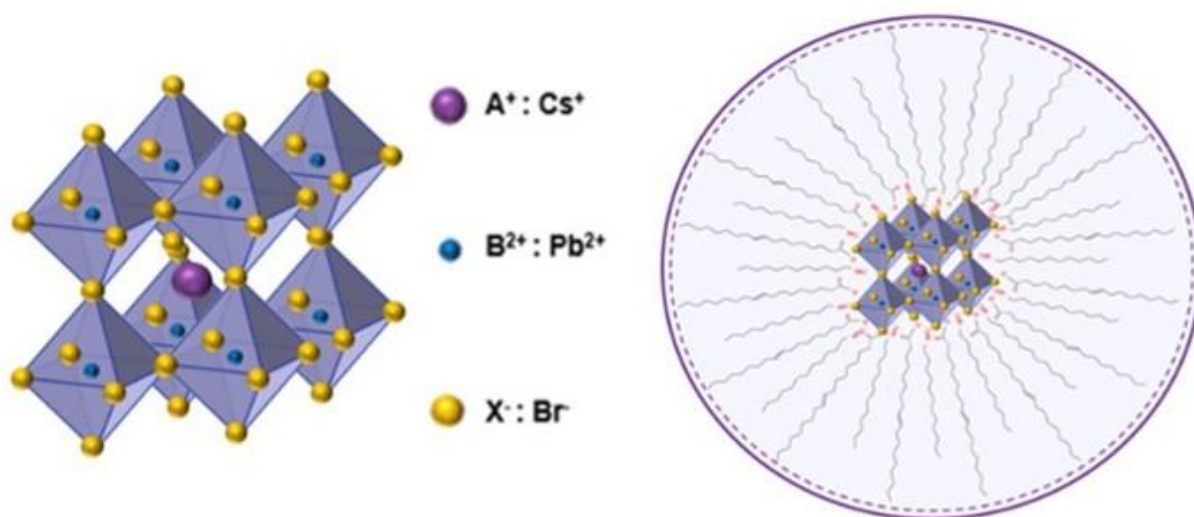
Despite these very interesting contributions, there are still many open or debatable questions to be addressed. If it is true that liquid NMR can be used to apprehend the labile nature of the native ligand with the presence of bounded, adsorbed and free species, it cannot be used to report on the surface termination and the ligand positioning. The surface termination of the $CsPbBr_3$ NCs, whether it is {Cs, Br}, {Pb, Br} terminated, or rather an ill-defined structure, is

still unclear. For instance, the presence of Cs vacancies and its relationship with the positioning of the bound ligands (oleyammonium / carboxylate), and whether the later are pairing on the surface is clearly lacking experimental data. In this internship, we propose to develop Dynamic Nuclear Polarization (DNP) enhanced solid-state NMR applied to perovskite nanocrystals, with the goal to answer such open questions. Even if DNP has revolutionized the NMR sensitivity and has been shown suitable to polarize various type of systems, polarizing perovskite nanocrystals has proven very challenging using standard equipment operating at 100 K. We will first investigate the best procedure to prepare the perovskite NCs for DNP measurements, given that the native ligands are extremely labile and that the purification and sample preparation steps might significantly modify the ligand/core interface and possibly even the NC surface termination. We will then test the performance of the latest generation of polarizing agents developed in our laboratory,[6–7] combined with measurements conducted at very low temperatures (30 K). These latest measurements are made possible by unique instrumentation worldwide, developed in-house.[9]

Master student profile and qualifications:
This project suits candidates following a master in Chemistry / Physical Chemistry / Materials science / Engineering with a strong interest in NMR spectroscopy. Knowledge in perovskite chemistry is not required but will be a plus. Excellent communication skills in English and the ability to work in a research team are required.

How to Apply:
Interested candidates should send a short motivation letter, a CV and transcripts of grades (License, M1) to Subhradip Paul (CEA Researcher, subhradip.paul@cea.fr) and Gaël De Paëpe (CEA Research Director, gael.depaepe@cea.fr).

Scientific environment and workplace:
The successful candidate will join the Magnetic Resonance laboratory at the Interdisciplinary Research Institute of Grenoble (IRIG). The laboratory is composed of five permanent researchers/assistant professors, one research-engineer, one technician, and multiple PhD students and postdocs. It hosts three research-oriented NMR spectrometers (200 / 400 / 500 MHz) equipped with state-of-the-art solution NMR, PFG, HRMAS and solid-state NMR probes. Furthermore, the laboratory is equipped with advanced solid-state NMR equipment, including two MAS-DNP systems, a home-built sustainable helium sample spinning system for ultra-low temperature MAS NMR and DNP, and an operando NMR setup for battery studies. The originality of the RM lab lies in the diversity of its research, which encompasses method development and major instrumental developments, but also advanced applications in battery research, functional materials, and complex biomolecular systems.
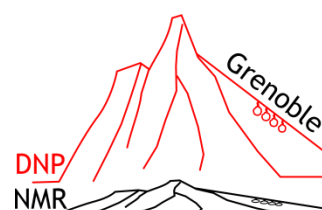
The Magnetic Resonance laboratory is part of the Modeling and Exploration of Materials Laboratory (MEM), a joint research unit of the CEA and the Université Grenoble Alpes. The MEM belongs to the Interdisciplinary Research Institute of Grenoble (IRIG), which gathers 10 laboratories and around 1000 researchers, technicians, doctoral and post-doctoral students,

covering a large variety of interdisciplinary fields (nanophysics, chemistry for health and energy, cryo-technologies, biology and medicine). Besides, IRIG includes also the IBS NMR groups, which are specialized in structural biology and host six NMR instruments, including a 950 MHz spectrometer. This strong environment in NMR is ideally complemented by research teams specialized in EPR, advanced electron microscopy, X-ray (lab equipment and ESRF) and neutron diffraction (ILL).

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More information about the group here and here.
More information about the IRIG institute here.

References related to the topic:

1- Protesescu, L. *et al.* Nanocrystals of Cesium Lead Halide Perovskites (CsPbX3, X = Cl, Br, and I): Novel Optoelectronic Materials Showing Bright Emission with Wide Color Gamut. *Nano Lett* **15**, 3692–3696 (2015).

2- Pan, J. *et al.* Highly Efficient Perovskite-Quantum-Dot Light-Emitting Diodes by Surface Engineering. *Advanced Materials* **28**, 8718–8725 (2016).

3- De Roo, J. *et al.* Highly Dynamic Ligand Binding and Light Absorption Coefficient of Cesium Lead Bromide Perovskite Nanocrystals. *ACS Nano* **10**, 2071–2081 (2016).

4- Smock, S. R., Williams, T. J. & Brutchey, R. L. Quantifying the Thermodynamics of Ligand Binding to CsPbBr3 Quantum Dots. *Angewandte Chemie* **130**, 11885–11889 (2018).

5- Chen, Y. *et al.*, Surface Termination of CsPbBr3 Perovskite Quantum Dots Determined by Solid-State NMR Spectroscopy. *J Am Chem Soc* **142**, 6117–6127 (2020).

6- R. Harrabi *et al.*, Highly Efficiency Polarizing Agents for MAS-DNP of Proton-Dense Molecular Solids, *Angew. Chem. Int. Ed.* **61**, e202114103 (2022).

7- Halbritter *et al.*, PyrroTriPol: a semi-rigid trityl-nitroxide for high field dynamic nuclear polarization, *Chem. Sci.* **14**, 3852 (2023).

8- S. Paul et al. Sustainable and cost-effective MAS DNP-NMR at 30 K with cryogenic sample exchange. *Submitted*

Projet bibliographique - Stage de recherche M2

Dynamic Nuclear Polarization of paramagnetic solids

**Contact gael.depaepe@cea.fr**

Project description:

Paramagnetic transition metal complexes are central to biological, chemical and physical sciences. Their unique properties are key in processes such as the respiratory cycle[1] and photosynthesis[2]. At the same time, they have gathered major interest for applications in catalysis and nanotechnology. The primary reason for their versatility being the unpaired electrons of the transition metal ions.

To understand their function, a suitable sets of characterization techniques is crucial. Oftentimes, it relies on the use of X-ray and neutron diffraction, electron microscopy and magnetic measurements. Despite the power of these techniques, they are unable to give insight into the electronic structure of individual atoms and how the unpaired electrons delocalize through the molecular system.

Solid-state paramagnetic nuclear magnetic resonance (pNMR)[3] is currently emerging as a key technique to probe the structure and electronic properties of such materials at an atomic level. In particular, the use of ultra-fast Magic Angle Spinning (MAS) of the sample, in combination with the design of tailored NMR pulse sequences has been shown to improve significantly the quality of the data (resolution and sensitivity),[3] and has enabled the detection of abundant nuclei (^1H, ^{31}P) and to some extent less receptive nuclei (e.g. ^{13}C).

The current pNMR approach that relies on the ability to accumulate a large number of transients is nevertheless not sufficient for more challenging nuclei such as ^{15}N and ^{17}O, mostly because of their incredibly low natural abundance (0.368% for ^{15}N, 0.038% for ^{17}O) and low gyromagnetic ratio. Hence, we propose to develop a novel approach based on the use of Dynamic Nuclear Polarization (DNP) and ultra-low temperature.[4,5] DNP has so far been successfully applied to hyperpolarize diamagnetic organic and inorganic solids, through the use of organic dopants (e.g. bisnitroxides)[6] and metal ions dopants (Mn^{2+} and Gd^{3+}),[7] but never to polarize a paramagnetic molecular solids. The work will be carried out on a prototypical mononuclear manganese (III) complex, with great potential for memory device applications,
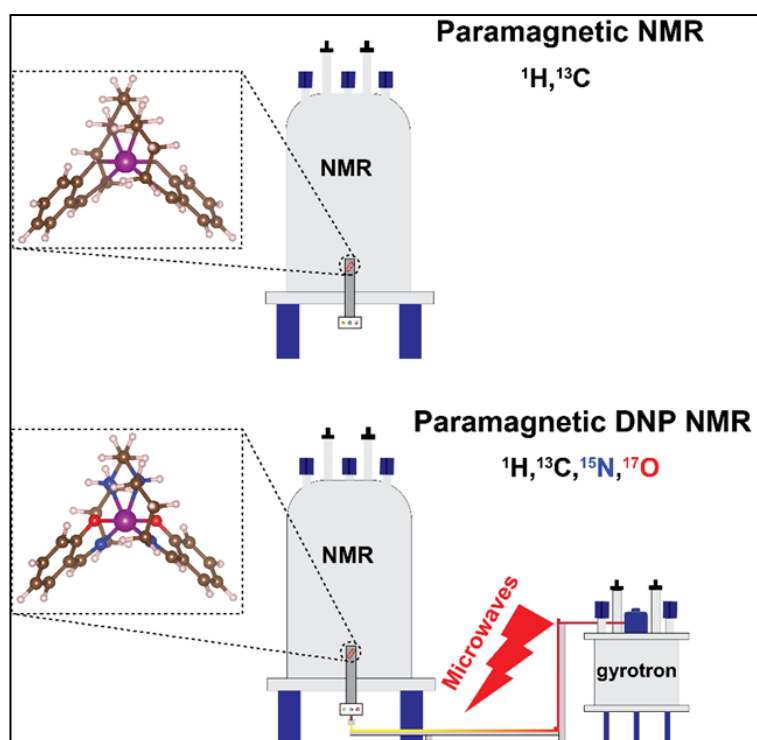
since it undergoes an electron spin transition around 130 K.[8] The candidate will employ state-of-the-art methodology and DNP equipment, to push the detection boundaries of these challenging nuclei in paramagnetic systems. This includes the access to a novel He-spinning instrumentation[9] (unique worldwide) that enables experiments at ultra-low temperatures (30K). The candidate will also be trained in quantum chemistry calculations of paramagnetic shifts[10] to aid the assignment of the obtained spectra.

Master student profile and qualifications:
This project suits candidates following a master in Chemistry / Physical Chemistry / Materials Science, Physics or Engineering with a strong interest in NMR spectroscopy and *ab initio* calculations. Excellent communication skills in English and the ability to work in a research team are required.

How to Apply:
Interested candidates should send a short motivation letter, a CV and transcripts of grades (License, M1) to Gaël De Paëpe (CEA Research Director, gael.depaepe@cea.fr).
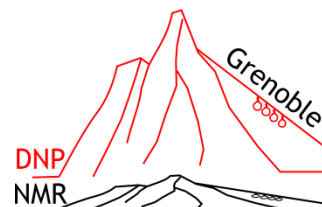
Scientific environment and workplace:
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More information about the group here and here.
More information about the IRIG institute here.

References related to the topic:

1. D. Kinschel, *et al.* Femtosecond X-ray emission study of the spin cross-over dynamics in haem proteins. *Nat Commun* **11**, 4145 (2020).

2. A. Bhowmick, *et al.* Structural evidence for intermediates during O2 formation in photosystem II. *Nature* **617**, 629-636 (2023).

3. A. J. Pell, G. Pintacuda, C. P. Grey, Paramagnetic NMR in solution and the solid state. *Progress in Nuclear Magnetic Resonance Spectroscopy* **111**, 1–271 (2019).

4. F. Mentink-Vigier, *et al.* Computationally Assisted Design of Polarizing Agents for Dynamic Nuclear Polarization Enhanced NMR: The AsymPol Family. *J. Am. Chem. Soc.* **140**, 11013–11019 (2018).

5. E. Bouleau, *et al.* Pushing NMR sensitivity limits using dynamic nuclear polarization with closed-loop cryogenic helium sample spinning *Chem. Sci.* **6**, 6806 (2015)

6. R. Harrabi, *et al.* Highly Efficient Polarizing Agents for MAS-DNP of Proton-Dense Molecular Solids. *Angew. Chem. Int. Ed.* **61**, e202114103 (2022).

7. T. Wolf, *et al.* Endogeneous Dynamic Nuclear Polarization for Natural Abundance 17O and Lithium NMR in the bulk of Inorganic Solids, *J. Am. Chem. Soc.* **141**, 1, 451-462 (2019)

8. P. N. Martinho, *et al.* Cooperative Spin Transition in a Mononuclear Manganese(III) Complex. *Angew. Chem. Int. Ed.* **51**, 12597–12601 (2012).

9. S. Paul, *et al.* Sustainable and cost-effective MAS DNP-NMR at 30 K with cryogenic sample exchange. ***Submitted***

10. J. Vaara, S. A. Rouf, & J. Mareš, Magnetic Couplings in the Chemical Shift of Paramagnetic NMR. *J. Chem. Theory Comput.* **11**, 4840–4849 (2015).

Projet bibliographique - Stage de recherche M2

Resonance assignment of *Sel*DNP spectra of proteins

Contact sabine.hediger@cea.fr and gael.depaepe@cea.fr

Project description:

In the last few years, our group introduced and developed an innovative approach, enabling the simplification of crowded 2D ^{13}C-^{13}C NMR spectra of proteins. Rather than containing cross-peak contributions from hundreds of residues present in the protein, *Sel*DNP spectra are restricted to about 30 residues, which are located within 20 to 30 A from a user-defined location (e.g. a protein binding site, or any residue from the protein).
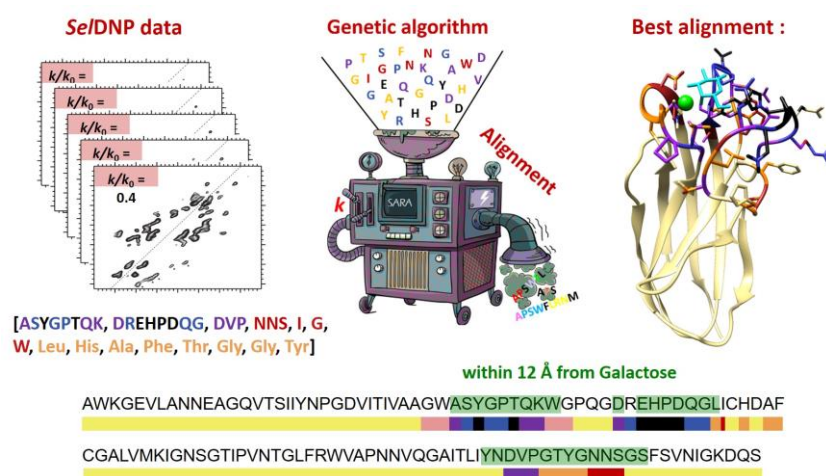
This method called *Selective* DNP (*Sel*DNP) is highly sensitive since it makes use of DNP hyperpolarization, while producing localized 2D datasets of only tens of residues. This approach circumvents one of the major drawback of using DNP for biomolecular systems. *Sel*DNP provides not only localized and hyperpolarized information of a given sub-part of a biomolecular system, but it also fixes the main problem currently limiting the broad application of DNP to a wide range of biomolecular systems. Indeed, DNP experiments generally require cooling the sample to cryogenic temperatures, which results in a line broadening of each NMR resonance and typically produces poorly resolved 2D data sets of hundreds of overlapping resonances. This limits the size of the biomolecular system that can be studied and imposes the use of *expensive* and *time-consuming* (segmental/methyl/etc.) isotopic labeling strategies. On the other end, *Sel*DNP does not have any size limitation and can be applied to *easy-to-produce* uniformly labeled ^{15}N, ^{13}C systems.

Whereas the type of the amino acids detected in *Sel*DNP spectra can easily be identified through the specific chemical shifts of sidechains carbons, their location on the protein sequence is difficult to assess due to the lack of experimental inter-residue information. Based on preliminary work from our group (*unpublished*), we believe that one can automatically assign the 30 residues contained in the *Sel*DNP spectra (mostly in the form of 2 to 4 segments from the protein sequence). A first attempt, based on the use a genetic algorithm, to align the detected residues on the protein sequence is very promising, but still limited. This internship will consist in improving the efficiency and the robustness of the algorithm by introducing additional

inherent distance information that are contained in *Sel*DNP spectra. The result will be tested using experimental data (already available in the lab), and simulated data (from proteins with known assignment from the Biological Magnetic Resonance Data Bank (BRMB). Specifically, large proteins and proteins with repeating motifs will be tested to interrogate the limits of the algorithm and suggests direction of improvement. In addition to the computational work, the candidate will be trained in DNP-enhanced solid-state NMR and more specifically will participate in *Sel*DNP experiments.

Master student profile and qualifications:
This project suits candidates following a master in Chemistry / Biochemistry / Physical Chemistry / Biophysics or Engineering with a strong interest in NMR spectroscopy. Knowledge in computer programming (Matlab, Python etc.) is required, as well as excellent communication skills in English and the ability to work in a research team.
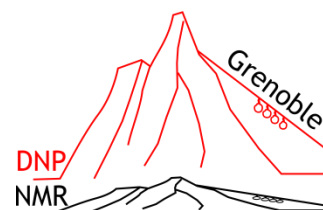
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CEA – Université Grenoble Alpes
Institut de Recherche Interdisciplinaire de Grenoble

Located in the French Alps and surrounded by a stunning natural environment, the international city of Grenoble represents an extremely rich ecosystem formed by public research organizations (CEA, CNRS, ESRF, ILL) and high-tech companies.

In addition, the Université Grenoble Alpes attracts a large number of students who can benefit from high-level academic training in a broad range of disciplines.

More information about the group here and here.
**More information about the IRIG institute here.**

References related to the topic:

1- I. Marin-Montesinos, D. Goyard, E. Gillon, O. Renaudet, A. Imberty, S. Hediger, & G. De Paëpe (2019). Selective high-resolution DNP-enhanced NMR of biomolecular binding sites. *Chemical Science*, *10*(11), 3366–3374. https://doi.org/10.1039/C8SC05696J

2- D. Gauto, O. Dakhlaoui, I. Marin-Montesinos, S. Hediger, & G. De Paëpe (2021). Targeted DNP for biomolecular solid-state NMR. *Chemical Science*, *12* (18), 6223–6237. https://doi.org/10.1039/d0sc06959k

3- W. Y. Chow, G. De Paëpe & S. Hediger (2022). Biomolecular and Biological Applications of Solid-State NMR with Dynamic Nuclear Polarization Enhancement. *Chemical Reviews*, *122* (10), 9795–9847. https://doi.org/10.1021/acs.chemrev.1c01043

4- O. Dakhlaoui, T. Halbritter, D. Gauto, E. Gillon, V. Chazalet, A. Varrot, A. Imberty, S. Th. Sigurdsson, S. Hediger & G. De Paëpe, Selective DNP of biomolecules with Site Directed Spin Labeling. *in preparation*

5- O. Dakhlaoui, D. Gauto, E. Gillon, A. Varrot, A. Imberty, S. Hediger & G. De Paëpe, Selective DNP of protein binding sites with diamagnetic ion. *in preparation*

Theoretical modeling of noise in hybrid quantum systems and devices

During this internship, we will apply novel theoretical tools to describe the effects of noise in quantum systems and devices. Some of such systems are being currently built and investigated in the framework of the Quantum Silicon initiative in Grenoble (https://www.quantumsilicon-grenoble.eu/), see also the figure below showing some of my works. This consortium brings together many experimentalists and theorists, also outside Grenoble, collaborating with the challenging goal to develop quantum technologies, also able to perform quantum simulation or computation. Many fundamental and practical questions have still to be addressed and solved on the theory side to guide ongoing experiments. In particular, it is still an open question to assess how quantum measurements and environmental noise affect such systems and can be even exploited to perform useful operations. This theoretical research will definitely have an impact on "real" experiments and your work will be constantly discussed with a variegated group of scientist with experimental and theoretical backgrounds.
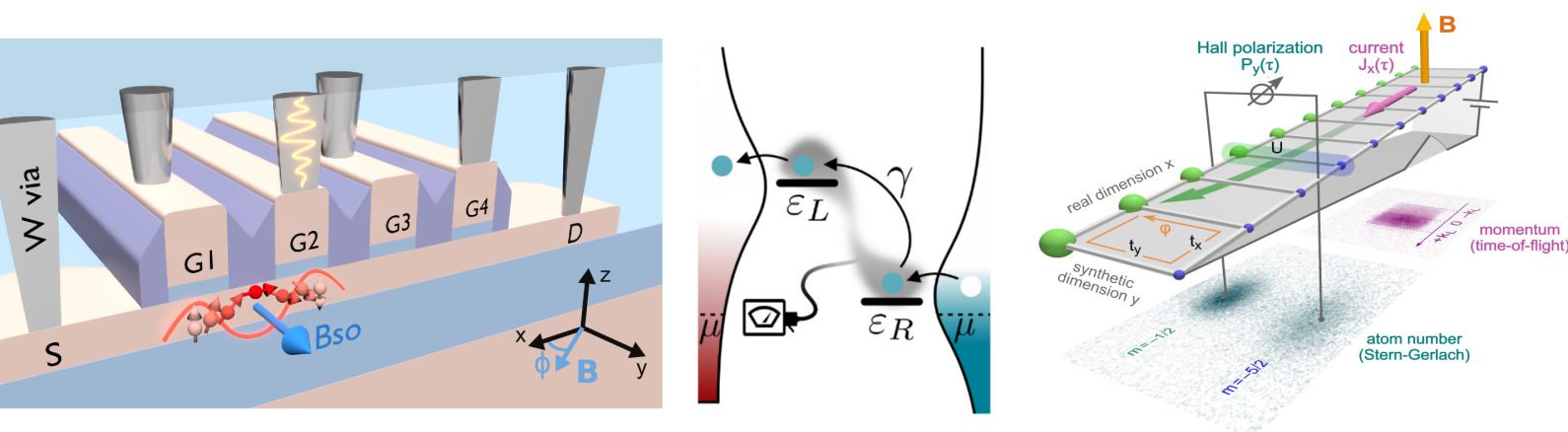
[1] Yu *et al.* Strong coupling between a photon and a hole spin in silicon **Nat. Nano.** (2023) [2] Ferreira *et al.* Exact description of transport in monitored quantum devices **arXiv** (2023) [3] Zhou *et al.* Observation of universal Hall response in strongly interacting Fermions **Science** (2023)

During this internship, you will deepen your knowledge of the rapidly developing fields of many-body quantum systems, material science and quantum matter and sharpen your analytical and numerical skills. These skills are strongly appreciated also outside academia.

For any question, do not hesitate to contact me at michele.filippone@cea.fr (some easy ones: what is in those pictures? and why should we care about? :))

Two words about myself as my internet site is not ready yet . . .

Hi! I am Michele Filippone and I am a new permanent theoretical researcher of the team L_Sim at the CEA–Grenoble. After my Ph.D. at the École Normale Supérieure of Paris and a Post-doc in Berlin, I have started my independent research activity in Geneva, where I have built my first research group. I have a longstanding interest in the description of the dynamics of quantum circuits, where quantum coherence, entanglement, superconductivity, Coulomb interactions and other intriguing phenomena are simultaneously at work. During my past research activity, I have advised several young researchers and established multiple collaborations with various experimental groups (including Google) studying quantum devices, cold atoms and topological materials.

Stage de recherche M2

Modeling the dynamics of silicon/germanium spin qubits

Contact: ynique@cea.fr

Project description:

Silicon/Germanium spin qubits have made outstanding progress in the past two years [1, 2]. In these devices, the elementary information is stored as a coherent superposition of the spin states of an electron in a Si/SiGe heterostructure, or of a hole in a Ge/SiGe heterostructure. These spins can be manipulated electrically owing to spin-orbit coupling, and are entangled through exchange interactions, allowing for a variety of one- and two-qubit gates required for quantum computing and simulation. Grenoble is developing original spin qubit platforms on Si and Ge, and holds various records in spin lifetimes [3] and spin-photon interactions [4].

At IRIG/MEM, we support the progress of these advanced quantum technologies with state-of-the-art modelling [3, 4]. In particular, we are developing the TB_Sim code, able to describe very realistic qubit structures down to the atomic scale if needed. **The aim of this master training is to model the quantum dynamics of single and coupled Si/Ge spin qubits in relation with recent experiments, using a combination of analytical and numerical (TB_Sim) techniques [1, 2]**.

This Master thesis may be followed by a PhD project that will address spin manipulation and entanglement in arrays of spin qubits, the response to noise and disorder (decoherence), and the interactions with photons (circuit quantum electrodynamics). The Master/PhD candidate will have the opportunity to interact with a lively community of experimentalists working on spin qubits at CEA and CNRS.
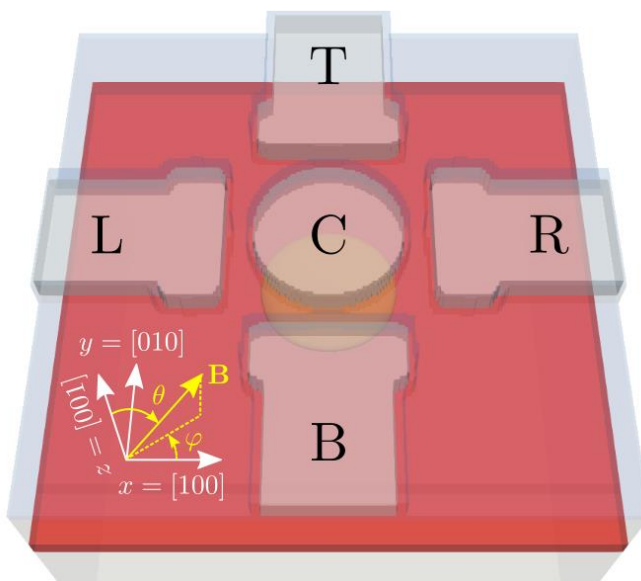
Model for a Germanium spin qubit: A quantum dot is shaped in a Germanium quantum well (red) by the potentials applied to the C/L/R/T/B gates. The up and down spin states of the hole trapped in this quantum dot are split by the magnetic field B *and used as a basis for coherent superpositions. The yellow shape is the isodensity surface that encloses 90% of the charge of the hole.*

Master student profile and qualifications:

The candidate must have a master in quantum or condensed matter physics/engineering, and a taste for numerical modeling. Excellent communication skills in English and the ability to work in a research team are required.

How to Apply:

Candidates should send a short motivation letter, a CV and transcripts of grades (License, M1) to Yann-Michel Niquet (yniquet@cea.fr).

Scientific environment and workplace:

The successful candidate will join the "Laboratory of Atomistic Simulation (L_Sim)" of the "Modeling and Exploration of Materials (MEM)" service of the Interdisciplinary Research Institute of Grenoble (IRIG). The group modeling spin qubits is composed of two permanent researchers, two PhD students and two postdocs. They work in very close collaboration with the members of the PHELIQS/LATEQS lab who measure these spin qubits.

More information about MEM here.
More information about the IRIG institute here.

References related to the topic:

[1] *A four-qubit germanium quantum processor*,
     N. W. Hendrickx *et al*., Nature **591**, 580 (2021) [arXiv:2009.04268].

[2] *Universal control of a six-qubit quantum processor in silicon*,
     S. G. J. Philips *et al.*, Nature **609**, 919 (2022) [arXiv:2202.09252].

[3] *A single hole spin with enhanced coherence in natural silicon*,
     N. Piot *et al*., Nature Nanotechnology **17**, 1072 (2022) [arXiv:2201.08637].

[4] *Strong coupling between a photon and a hole spin in silicon*,
     C. X. Yu *et al*., Nature Nanotechnology **18**, 741 (2023) [arXiv:2201.08637].

Stage de recherche M2

Atomic structural characterization of new single-layer 2D materials

Contact mahesh-krishna.prabhu@esrf.fr and gilles.renaud@cea.fr

Project description:
Discovering the synthesis strategies to new 2D materials and linking their atomic structure to physical and chemical properties that can open up new potential applications especially in green hydrogen, energy production and storage is a major forefront in modern physics. In this M2 project, We will investigate synthetic 2D transition metal dichalcogenides (TMDCs) of group 8-10 metals (e.g. Fe, Ni, Co, Ru) assuming the X-M-X structure encountered in MoS_2 and WS_2 natural crystals.[1] Synthesizing stable M-X-M 2D structure with these metals would further broaden the application potential of 2D TMDCs,[2-4] towards spintronics, piezoelectricity, optics, photovoltaics, photocatalysis and fuel cells.[6] The 2D TMDCs will be synthesized by a physical vapor deposition (PVD) process in ultra-high vacuum (UHV) experimental setups. The investigations will be carried out using synchrotron techniques like *in situ* grazing incidence surface X-ray diffraction and combined with other techniques such as reflection high-energy electron diffraction (RHEED), Auger electron spectroscopy (AES), scanning tunneling microscopy (STM) and low energy electron diffraction (LEED). The experiments will involve the use of facilities of the beamline BM32 at ESRF and laboratory facilities of Néel Institute (Grenoble). The data analysis by combining all of the experimental data will be performed to determine the atomic structure of the 2D materials along with their physicochemical properties. For example, by combining the diffraction data with the chemical compositions inferred from AES, we will unveil how the atomic structure of the new 2D materials depend on the metal and chalcogen composition. From the in-plane and perpendicular atomic displacements associated with moiré patterns, we will also gain fine insights into the nature of interactions with the substrate used for the growth. Our project prompts more fundamental questions, for instance, if it is possible to force any transition metal to adopt a layered TMDC structure on the basis of the substrate interaction stabilizing the atomic structure. Finding answers to such fundamental question on new 2D material synthesis is a gateway to the discovery of new 2D TMDCs, with foreseeable applications exploiting catalytic, magnetic, piezoelectric, optical and electronic conduction properties.

Master student profile and qualifications:
This project suits candidates following a master in Chemistry / Physical Chemistry / Materials science / Engineering with good background of basic surface science, condensed matter physics or solid state chemistry. Having a strong interest in working with experimental techniques 'hands-on' is important for this M2 project. Good communication skills in English and the ability to work in a research team are required.

How to Apply:
Interested candidates should send a short motivation letter, a CV and transcripts of grades (License, M1) to Mahesh-Krishna PRABHU (CEA Researcher, **mahesh-krishna.prabhu@esrf.fr**) and Gilles RENAUD (CEA Scientist, **gilles.renaud@cea.fr**)

Scientific environment and workplace:
The successful candidate will join the research team of the Interdisciplinary Research Institute of Grenoble (IRIG) working at the CRG-IF beam-line (BM32) at ESRF. The CRG-IF beam-line is jointly operated by the Centre National de la Recherche Scientifique (**CNRS**) and the Commissariat à l'Energie Atomique et aux Energies alternatives (**CEA**). The research team is composed of several scientists and postdocs from both CEA and CNRS working on a broad range of research topics. The INS2 hutch of BM32 offers a UHV system to perform *In-situ* study of atomic layers growth by means of **scattering X-ray techniques from 5 to 27 keV.** In INS2, the growth of nanometric films, particles, nanowires or new 2D material is achieved using a combination of techniques including molecular beam epitaxy (MBE) and chemical vapor deposition (CVD). X-ray measurements allow for *in situ* structural studies on the atomic scale by grazing incidence scattering at large angles (GIXS/GIXD/SXRD/XRR) and morphological studies on the scale of a few nanometers or tens of nanometers, by scattering at small angles in grazing incidence (GISAXS). The research work carried out at BM32 is complemented by the experimental support from the UHV setups at the Néel Institute, which is a part of the CNRS.

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More information about the scientific environment and the research group can be found here : https://www.esrf.fr/UsersAndScience/Experiments/CRG/BM32
More information about the IRIG institute here.

References related to the topic:
(1) Nat Rev Mater 2017, 2, 17033; (2) Nano Energy 2015, 18, 293-305; (3) Biomaterials. 2021, 269, 120471; (4) Adv. Mater. Interfaces 2019, 6, 1901329. (5) Journal of Phy. Chem. C 2012, 116 (16), 8983–8999; (6) Adv. Funct. Mater. 2020, 30, 1903929;

Stage de recherche M2

Strain, defects and interfaces in advanced microelectronics substrates using synchrotron X-ray techniques

Contact samuel.tardif@cea.fr

Project description:

This project is at the cross-road of technological innovation, fundamental physics and materials science & engineering, with a background of large-scale research facilities.

The context of the project is the current necessity for faster, more energy efficient and cheaper devices, which drives the research for new materials and processes. This is particularly important in the field of power electronics and optoelectronics to support the ongoing energy transition. Several wide bandgap semiconductors (SiC, GaN, and diamond) have been identified for their electronic and optical properties. These materials have wider operating ranges in temperature, frequency, and voltage, as well as better electrical conversion efficiencies than the current solutions. Their optical properties also make them excellent candidates for integrated optoelectronics. However, the manufacture of substrates for the realization of electronic devices from these materials is complex, expensive, and energy-intensive. In order to fully benefit from their large-scale application, it is necessary to develop a more frugal and optimized process.

To that end, the SmartCut™ technology is very suitable, as it can produce substrates by thin-film transfer. SmartCut™ is a technology developed at the CEA, transferred to the French company SOITEC, and currently widely used for the production of Silicon-on-Insulator (SOI) substrates. This technique consists in cutting sub-micrometer "slices", for example from high-quality wafers up to 300 mm in diameter, and transferring them onto receiving substrates, possibly with different properties or lower cost. The technology is based essentially on two fundamental mechanisms: (1) the direct bonding technique, and (2) the controlled fracture through a weakened layer. Direct bonding involves bringing two surfaces of potentially different but necessarily very flat nature into contact and creating covalent chemical bonds between them by mastering the thermal, mechanical, and physico-chemical properties of the interface. The fracture consists in separating the assembly by thermal annealing, that will mature microcracks in weakened layer until the propagation of a macroscopic fracture.

Although the SmartCut™ technology is currently widely used for silicon and the production of SOI, its application to other materials is still under development. Much is left to be understood about the different mechanisms involved at all stages of the transfer process on these new materials. There is a strong need to understand the physical phenomena at play, in particular what happens *at* and *through* the bonding interface, in terms of microstructure, strain and defects. The scope of the M2 internship is to use the microLaue technique available at the beamline and recently upgraded to study the relationship between the strain in the

transferred film and the underlying substrate (grain size, orientation). Possibly, the defects may also be investigated (type of defect, spatial extension…). The microLaue is a unique technique that provides local (sub-micron) information on the crystal structure: crystal orientation and lattice parameters. From the deviation of the lattice parameters to the ideal relaxed state, the local crystalline strain can be computed. The data acquisition being relatively fast (on the order of 1 s/pt), extended maps can be recorded. Preliminary data has already been collected for novel substrates made of single crystal SiC transferred on polycrystalline SiC. Additional synchrotron measurement campaign(s) are foreseen. The data analysis software is developed by our research team and available open-source. The course of the project thus goes through successive goals, from the analysis of previously acquired data, running new experiments at the synchrotron to acquire missing data, using/developing data analysis tools to extract physical quantities from experimental data, and up to building physical models of the underlying mechanisms based on the relationships between the different properties measured.

A possible extension to a PhD project can further be discussed.

Master student profile and qualifications:

This project suits candidates following a master in Materials Science & Engineering / Physics with some background on crystallography, condensed matter physics and/or mechanics. Having a strong interest in working with experimental techniques 'hands-on' is important for this M2 project. Good communication skills in English, the ability to work in a research team and an intermediate level in Python are required.

How to Apply:

Interested candidates should send a short motivation letter, a CV and transcripts of grades (License, M1) to Samuel Tardif (CEA Researcher, samuel.tardif@cea.fr).

Scientific environment and workplace:

The successful candidate will join the research team of the Interdisciplinary Research Institute of Grenoble (IRIG) of the Commissariat à l'Energie Atomique et aux Energies alternatives (CEA), operating the CRG-IF beamline (BM32) at ESRF jointly with the Centre National de la Recherche Scientifique (CNRS). The research team is composed of scientists and postdocs from both CEA and CNRS working on a broad range of research topics. The BM32 beamline is currently being upgraded, with new optics planned for installation before 2024. The Laue microdiffraction setup is also being upgraded at the beamline. The team at IRIG works in close collaboration with the CEA LETI ("Laboratoire d'Electronique et des Technologies de l'Information") on the topic of the SmartCut technology, as well as with the SOITEC company.

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More information about the scientific environment and the research group here.
**More information about the IRIG institute here.**

Stage de recherche M2

Bragg coherent diffraction imaging of nanoparticles

Contact ewen.bellec@esrf.fr and mrichard@esrf.fr

Project description:

The goal of this internship is to study the evolution of the structure (composition, defects, displacement and deformation field, *etc*.) of individual nanoparticles during catalytic reactions.
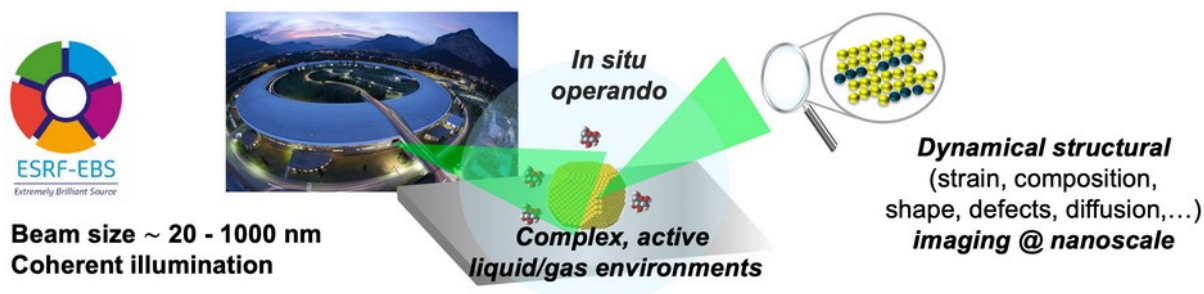
To achieve this, the student will apply the unique capabilities of Bragg Coherent Diffraction Imaging (BCDI) [1] using x-rays in a synchrotron environment. Due to its high spatial resolution ($\approx$ 5-10 nm^3) and excellent sensitivity to atomic displacements and local strain [2–4], Bragg coherent diffraction imaging has become a powerful tool over the past two decades for probing the three-dimensional (3D) structure and local deformation field within particles ranging from 50 nm to 1 μm in diameter. This non-destructive technique is particularly relevant for *in situ* and *operando* studies of nanoparticles. It benefits from recent technological advancements, such as the "Extremely Brilliant Source" (EBS) Upgrade at the ESRF, the European synchrotron located in Grenoble. By utilizing the unique capabilities of BCDI, the student will map *in situ*, *operando* (during operation), and in 3D the structural response (*e.g.*, evolution of deformation field and crystallographic defects) of individual nanoparticles undergoing catalytic reactions. This technique paves the way for analyzing the internal structure of nanoparticles and optimizing them for catalytic reactions. The experiments will be conducted at the ESRF within a leading international scientific environment. The student will first be introduced to the basics of Bragg coherent diffraction for the study of nanomaterials and to its data treatment using the *bcdi* package [5] for pre- and post-processing and the *PyNX* [6] package for phase retrieval. The student will then work on datasets collected at The European synchrotron (ESRF) and participate in the development of Python scripts or use existing ones to get an improved spatial resolution or to retrieve the complex measured object from several Bragg reflections.

A possible extension to a PhD project can further be discussed.

Master student profile and qualifications:

This project suits candidates following a master in science. He/she will preferably have deepened knowledge in physics, chemistry, material science or closely related science. He/she should also have experience or show some interest in image processing and analysis program development using *e.g.* Python programming. He/she should have good interpersonal, communication, organisational and presentational skills. The working language is English.

How to Apply:

Interested candidates should send a motivation letter, a CV and transcripts of grades (License, M1) to Ewen Bellec (ewen.bellec@esrf.fr) and to Marie-Ingrid Richard (mrichard@esrf.fr).

Scientific environment and workplace:

The successful candidate will join the CARINE's research team (https://carine-erc.eu) at the Interdisciplinary Research Institute of Grenoble (IRIG) of the Commissariat à l'Energie Atomique et aux Energies alternatives (CEA). The team has been beneficiary of an European project grant (https://carine-erc.eu) and is composed of scientists, postdocs and PhD students. The work will be done in collaboration with the ID01 beamline of ESRF. The internship position is located at ESRF. The ESRF (European Synchrotron Radiation Facility, https://esrf.eu) is a multinational research institute, situated in Grenoble, France. It operates one of the most powerful synchrotron x-ray sources. Both institutes offer a highly dynamic, exciting and multinational working environment in the French Alps.

Located in the French Alps and surrounded by a stunning natural environment, the international city of Grenoble represents an extremely rich ecosystem formed by public research organizations (CEA, CNRS, ESRF, ILL) and high-tech companies. In addition, the Université Grenoble Alpes attracts a large number of students who can benefit from high-level academic training in a broad range of disciplines.

More information about the group here and here.
More information about the IRIG institute here.

References related to the topic:

[1]   I. Robinson and R. Harder, *Coherent X-Ray Diffraction Imaging of Strain at the Nanoscale*, Nat Mater **8**, 291 (2009).

[2]   J. Carnis et al., *Twin Boundary Migration in an Individual Platinum Nanocrystal during Catalytic CO Oxidation*, Nat Commun **12**, 5385 (2021).

[3]   M. Dupraz et al., *Imaging the Facet Surface Strain State of Supported Multi-Faceted Pt Nanoparticles during Reaction*, Nat Commun **13**, 1 (2022).

[4]   C. Atlan et al., *Imaging the Strain Evolution of a Platinum Nanoparticle under Electrochemical Control*, Nat. Mater. **22**, 6 (2023).

[5]   Jerome Carnis, *Carnisj/Bcdi: V0.0.5*, (2019).

[6]   V. Favre-Nicolin, G. Girard, S. Leake, J. Carnis, Y. Chushkin, J. Kieffer, P. Paleo, and M.-I. Richard, *PyNX: High-Performance Computing Toolkit for Coherent X-Ray Imaging Based on Operators*, J Appl Cryst **53**, 5 (2020).
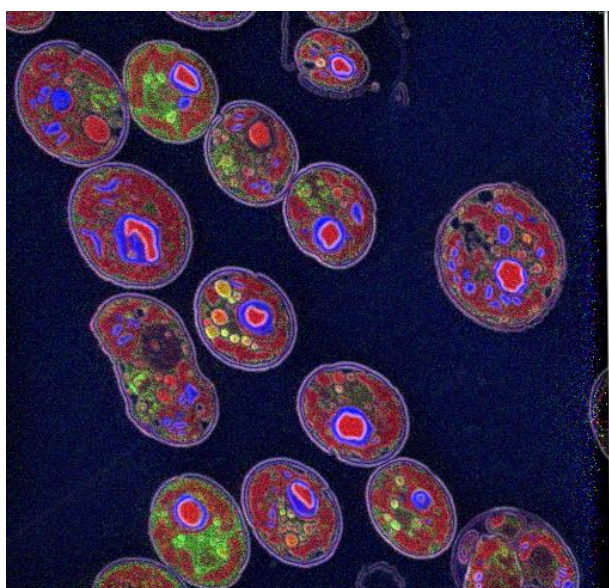
M2 internship – 6 months

Expansion microscopy for visualization of cellular compounds at the organelle level by mass spectroscopy imaging

Contact claire.seydoux@cea.fr and pierre-henri.jouneau@cea.fr

Project description:

The efficiency of biological organisms at performing a wide range of biochemical operations, ranging from e.g. cellular respiration, nutrient uptake, or degradation of toxic elements relies on the compartmentalization of such pathways into *(i)* specialized cells at the tissue level or *(ii)* specialized compartments named organelles at the subcellular level, typically of ~1 µm in size. When trying to study biological phenomena, a major challenge is the difficulty of knowing precisely the location of the molecule(s) involved.

Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) is a mass spectrometry imaging technique that produces chemical maps of elements and molecules up to ~1000 kDa with a lateral resolution up to ~50 nm by bombarding the sample with a focused ion beam and

Correlative ToF-SIMS/SEM imaging of microalgae cells. ToF-SIMS provides a full mass spectrum for every pixel, enabling untargeted molecular characterization of the sample. Selected ions were then chosen to display the subcellular content of the cell. The blue rings surrounding the intense red spots correspond to the pyrenoid of these alga, which is the locus for CO_2 fixation. Red: proteins. Blue: carbohydrates. Green: phosphates. Field of view: 50 µm, lateral resolution 100 nm. The proposed method is expected to enhance lateral resolution up to 25 µm in this case.

analyzing the sputtered ions in a mass analyzer (Fearn 2014, Fletcher 2015, Gilmore at al., 2019). Its use for the detection of biological molecules has been on the rise in the previous decades, however, it is currently limited mostly to the study of tissues since intrinsic reasons in the ionization method impose a trade-off between the mass of the molecule analyzed and the lateral resolution. Subcellular resolution is yet unachievable for large molecules such as full lipids or full drugs (Massonet et al., 2019, Bich et al., 2014).

Recently, the rapid and inexpensive technique of expansion microscopy has enabled unprecedented progress in routine imaging in the biological field. Briefly, this method consists
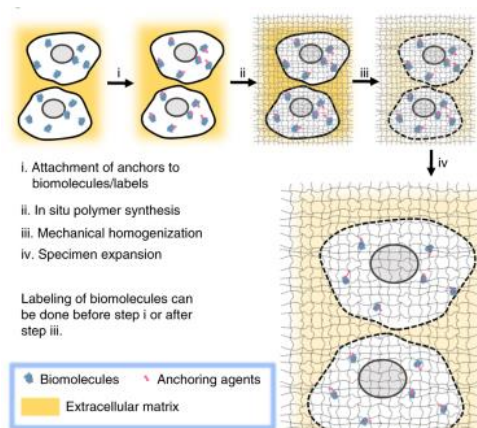
Principle of expansion microscopy. Adapted from Wassie et al, 2018

in expanding a given cell or tissue by a factor of ~4 through hydrogel polymerization inside the sample (Wassie et al., 2018), originally aiming at super-resolution light fluorescence microscopy. Recent articles have shown that modified versions of the classical protocols are compatible with mass spectrometry (Bai et al., 2023, Chan et al., 2023). It has not yet been applied to ToF-SIMS and we believe that this technique could render possible the subcellular localization of biomolecules such as lipids, carbohydrates or drugs and have a large impact over the capabilities of mass spectrometry imaging.

During this internship, we will be focusing on the green alga *Chlamydomonas reinhardtii*. Under some specific stress conditions, *Chlamydomonas* cells are able to accumulate large amounts of lipids in their cytoplasm that are of high interest for potential biofuel or dietary supplement (Li-Besson et al., 2015). However purifying these lipid droplets is a difficult task that takes up several days with high risks of contaminating the sample, and the contents of these droplets are yet difficult to analyze with current bulk mass spectrometry tools. Many tools, including a collection of mutant lines, are available for *Chlamydomonas* which make it a suitable organism for such prospective studies. With a size of ~10 µm, *Chlamydomonas* is too small for subcellular ToF-SIMS analysis of large molecular weight compounds, but expansion microscopy is a promising method to raise this barrier.

Master student profile and qualifications:
We are looking for a candidate following a master in e.g. Biology, Chemistry or Materials Science, but other domains can also be welcome. The main requirements for this project are to be interesting in imaging and in biology and to be willing to learn from new disciplines. This project is highly interdisciplinary and you will perform mass spectrometry imaging, sample preparation for biological organisms, analytical chemistry, electron microscopy, data analysis, cell biology, etc. thanks to the help provided by the diverse project team. The language can be either French or English depending on the student.

How to Apply:
Interested candidates should send a motivation letter and a CV to Claire Seydoux (claire.seydoux@cea.fr) and Pierre-Henri Jouneau (pierre-henri.jouneau@cea.fr). You can of course contact us if you have any questions. Please note that the security policy of CEA-Grenoble requires a 3-month waiting time between the moment an application is filled and its final approval, so make sure not to delay yours for too long.

Scientific environment and workplace:

You will be joining the Advanced Microscopy for Materials Study laboratory (LEMMA, CEA-Irig) in close collaboration with *(i)* the Surface and Interface Analysis laboratory (LASI, CEA-Leti) that holds a world-acknowledged experience in ToF-SIMS, *(ii)* the Electron Microscopy platform at the Institute of Structural Biology (MEM-IBS, CEA-Irig) for help with sample preparation, *(iii)* the Plant and Cell Physiology lab (LPCV, CEA-Irig) for supply of biological material and help with the expansion protocol. You will be closely supervised by Claire Seydoux, a post-doctoral researcher at LEMMA who is already developing ToF-SIMS imaging for biological cells and has now gained a good knowledge of the subject. You will be located at the PFNC, a highly international and friendly place to work composed of many researchers, postdocs and PhD students.

The city of Grenoble is surrounded by splendid mountains in the heart of the French Alps. It is also a very dynamic research city with ~10% of the city population working in research or R&D, many research labs and companies, and ~ 60,000 students in the University. It is as such a very nice place to be a student in.

References related to the topic:

Bai, Yunhao, et al. "Expanded vacuum-stable gels for multiplexed high-resolution spatial histopathology." *Nature Communications* 14.1 (2023): 4013.

Bich, C., Touboul, D., & Brunelle, A. (2014). Cluster TOF-SIMS imaging as a tool for micrometric histology of lipids in tissue. *Mass spectrometry reviews*, *33*(6), 442-451.

Chan, Yat Ho, et al. "Gel-assisted mass spectrometry imaging." *bioRxiv* (2023): 2023-06.

Fearn, S. "Characterisation of biological material with ToF-SIMS: a review." *Materials Science and Technology* 31.2 (2015): 148-161.

Fletcher, John S. "Latest applications of 3D ToF-SIMS bio-imaging." *Biointerphases* 10.1 (2015).

Gilmore, Ian S., Sven Heiles, and Cornelius L. Pieterse. "Metabolic imaging at the single-cell scale: recent advances in mass spectrometry imaging." *Annual review of analytical chemistry* 12 (2019): 201-224.

Li-Beisson, Yonghua, Fred Beisson, and Wayne Riekhof. "Metabolism of acyl-lipids in Chlamydomonas reinhardtii." *The Plant Journal* 82.3 (2015): 504-522.

Massonnet, Philippe, and Ron MA Heeren. "A concise tutorial review of TOF-SIMS based molecular and cellular imaging." *Journal of Analytical Atomic Spectrometry* 34.11 (2019): 2217-2228.

Wassie, Asmamaw T., Yongxin Zhao, and Edward S. Boyden. "Expansion microscopy: principles and uses in biological research." *Nature methods* 16.1 (2019): 33-41.

CEA – Université Grenoble Alpes
Institut de Recherche Interdisciplinaire de Grenoble

Stage de recherche M2

Mapping electric field in twisted 2D materials using 4D scanning transmission electron microscopy

Laboratory: LEMMA (IRIG/DEPHY/MEM- CEA Grenoble)
Contact: Hanako Okuno (hanako.okuno@cea.fr)

General scope:

Structural engineering of atomically thin two-dimensional (2D) materials, such as graphene, hexagonal boron nitride (h-BN) and transition metal dichalcogenides (TMDs), has become an exciting field of research to explore new and exotic quantum physics. For example, when two 2D layers are stacked with a small twist angle, a moiré pattern emerges due to the interference of the two crystal lattices. This moiré pattern alters the electronic and optical properties of the material by inducing additional local electrostatic potentials in a stack[1]. In order to understand and tailor such new phenomena, it is crucial to develop appropriate advanced characterization techniques. **Four-dimensional scanning transmission electron microscopy (4D STEM)** is a new STEM technique that allows to access the local electric field present at atomic length scales in a material. A focused electron probe is raster scanned over the sample, and a diffraction pattern is acquired at each probe position. The resulting dataset consists of 2D images in both real and reciprocal spaces, so-called 4D dataset. The presence of an (electric) field in the sample results in a deflection of the transmitted beam. Therefore, careful analysis of the transmitted beam position, using the Centre of Mass (CoM) approach, can give access to electric fields with atomic spatial resolution, and through Poisson's equation, to the charge density and electrostatic potential[2]. This technique opens a new STEM capability to probe structure-property relationships in 2D materials at the atomic scale.
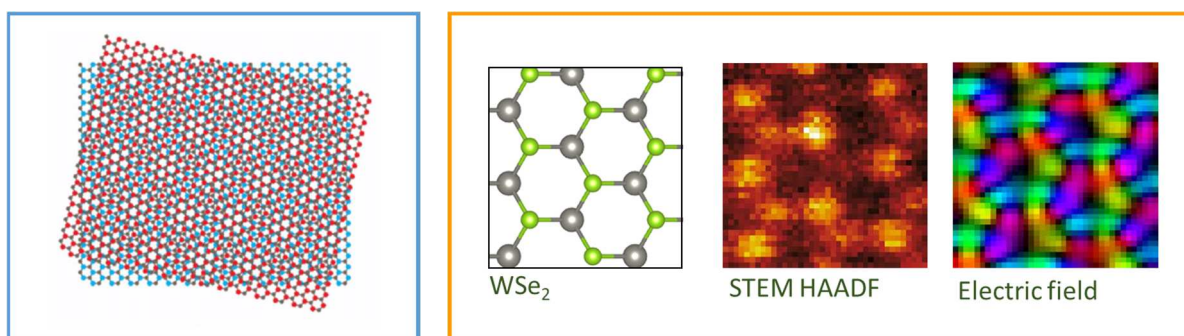
Figures: (left) schematic illustration of twisted bilayer with moiré pattern and (right) atomic resolution local electric field mapping of WSe$_2$ monolayer obtained by the CoM technique in the LEMMA group.

Project description:

Recently, the Laboratory of Advanced Electron Microscopy for Materials Study (LEMMA) has established a quantitative analytical process using the CoM to study the atomic scale electric field and potential induced by defects in atomically thin 2D monolayers[3]. **The aim of this internship** is to contribute to: i) the methodological optimization of the 4D STEM CoM method

for the electric field mapping of twisted bilayer systems and ii) the study of the nature of twisted bilayers by combining local structure-potential analysis. The student will prepare twisted bilayer TEM samples with different twist angles by a layer-by-layer technique already optimized in the group. He/she will assist in the 4D STEM experiments and data acquisition on a state of the art aberration corrected STEM. Then, he/she will analyze different data sets acquired on both single component monolayers and their twisted bi-layer stacks, using the CoM analysis protocol developed in the group. The internship work has access to various types of 2D materials (MoS_2, $MoSe_2$, graphene, WS_2 etc.) synthesized by the collaborators in other ongoing projects. **The goal of this internship** is to identify the electric field arising from structural moiré patterns. The results will open the possibility to extend the application of this technique to study many other structure-induced properties such as ferroelectricity.

Collaborations:

Spintec (CEA-IRIG) for the materials growth and properties and Institut Néel (CNRS) for the technical development.

Scientific environment and workplace:

The internship student will be hosted in the LEMMA of the IRIG institute situated at the CEA nanocharacterization platform (PFNC), which gives access a wide range of state-of-the art facilities including 3 probe aberration corrected microscopes (Titan Themis, double-corrected Titan Ultimate, JEOL NEO-ARM), equipped with GIF energy filter, monochromator and a direct electron detector. The group has a strong expertise on 1D and 2D materials study and is working in strong collaboration with several teams on growth, modelling and devices. The laboratory is located in the "Polygone Scientifique", near the city centre of Grenoble, which offers an exceptional working environment as well as a very good quality of life, in the heart of the French Alps.

Possible extension as a PhD:

Not granted in advance, but we are open to support applications for various PhD grants.

Required skills:

Interest in solid-state physics, materials sciences and engineering, advanced transmission electron microscopy and data analysis.

Starting date: Jan/Feb 2023 or earlier.

How to Apply:

Interested candidates should send a short motivation letter, a CV and transcripts of grades (Licence/bachelor, M1) to Hanako Okuno (hanako.okuno@cea.fr).

References related to the topic:

1. *Twistronics and the small-angle magic*, A. Jorio, Naturematerials, 21, 844 (2022)
2. *Sub-Angstrom electric field measurements on a universal detector in a scanning transmission electron microscope,* J. A. Hachtel et al., Adv. Struc. And Chem. Imaging, 4, 10 (2018)
3. *Atomic scale imaging of the negative charge induced by single vanadium dopant atom in monolayer WSe_2 using 4D-STEM*, D. Dosenovic et al., to be submitted.

https://www.mem-lab.fr/en/Pages/LEMMA/STEM.aspx (2D activities in LEMMA)
https://www.mem-lab.fr/en/Pages/LEMMA/Presentation.aspx (LEMMA laboratory)