PhD position | Chiral metal halides for photonics and spintronics

Contract	Fully funded 3-year PhD position
Starting date	October 2024
Gross monthly salary	2 135 €
Institution	Institut des Sciences Chimiques de Rennes (ISCR)
Contact	Dr. Mikaël KEPENEKIAN, Email: mikael.kepenekian@univ-rennes.fr

A full-time 3-year PhD position, starting October 2024, is available in the Theoretical Inorganic Chemistry team at the Institut des Sciences Chimiques de Rennes (ISCR, France) under the supervision of Dr. Mikaël Kepenekian. The project is dedicated to the characterization and design, using quantum chemistry approaches, of the photonic and spintronic properties of metal halides incorporating chiral cations.

Over the past decade, metal halides, and in particular halide perovskites, have experienced a resurgence of interest, giving rise to a new family of photovoltaic devices with record performances exceeding those of silicon-based solar cells. Interestingly, those materials offer great structural diversity, especially when moving away from the original all-inorganic structures to hybrid organic-inorganic metal halides, where larger organic molecules act as cations. This flexibility enables the incorporation of chiral ligands, which allow perovskites to be used in chiroptoelectronic, and chiro-spintronic applications, aided by measured long spin lifetimes.

Since 2017 and the first chiroptical studies of chiral halide perovskites, the field has grown rapidly and many flavors have been synthesized and characterized in various ways (**Figure 1**). The compounds are then used for various applications, such as circularly polarized photo-detectors and light sources. Importantly, light wave with chiral features are expected to play a major part in high-bandwidth optical communication and cryptography. In addition, chiral metal halides might be of great interest in spintronics, taking advantage of the recently evidenced ability of chiral systems to inject or detect spin currents through the chiral-induced spin selectivity (CISS).

While examples of chiral halogenated perovskites are multiplying, the mechanisms for transferring chi-

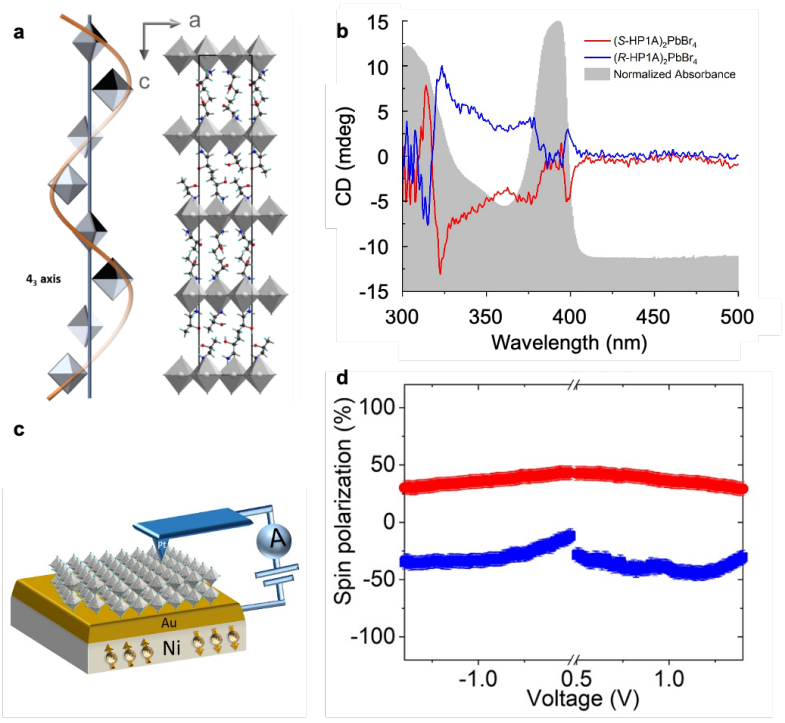


Figure 1 | Example of optical and spin characterizations of a chiral halide perovskite [1]. **a** Crystal structures of $(S\text{-HP1A})_2PbBr_4$ with illustration of the 4_3 and 4_1 symmetry elements. **b** Circular dichroism and absorbance spectra of thin films of $(S\text{-HP1A})_2PbBr_4$ and $(R\text{-HP1A})_2PbBr_4$. **c** Schematic representation of the magnetic conducting atomic force microscopy (mc-AFM) measurements. **d** Average values of spin polarization in $(S\text{-HP1A})_2PbBr_4$ (red) and $(R\text{-HP1A})_2PbBr_4$ (blue).

rality from the cation to the inorganic framework have yet to be identified. The successful candidate will undertake the description, using electronic structure and optical property calculations based on density functional theory (DFT) and complemented by semi-empirical approaches, of chiral halide perovskites synthesized and characterized by our collaborators Dr. A. Abhervé (MOLTECH-Anjou), Prof. F. Deschler (University of Heidelberg), as well as our long standing collaborators from the USA Prof. M. G. Kanatzidis (Northwestern University) and Prof. A. D. Mohite. This methodological leap forward pursued in close collaboration with experimental teams, will enable us to establish the design rules for future systems with optimum performance.

Related references

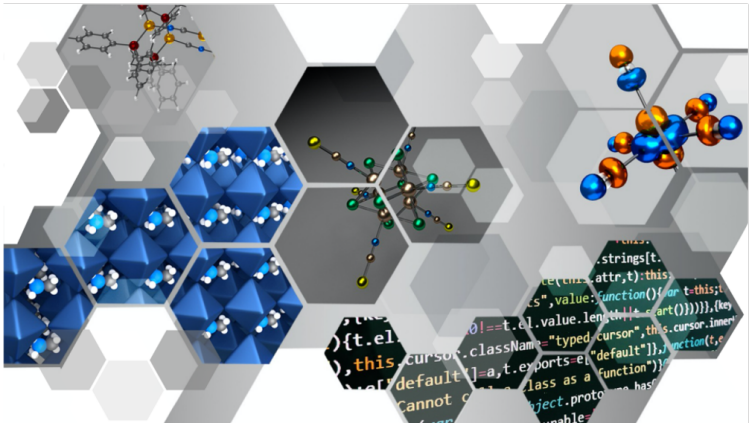
[1] A. Abhervé, N. Mercier, A. Kumar, T. K. Das, J. Even, C. Katan, M. Kepenekian, *Adv. Mater.* **2023**, *35*, 2305784 HAL

[2] S. Liu, M. Kepenekian, S. Bodnar, S. Feldmann, M. W. Heindl, N. Fehn, J. Zerhoch, A. Shcherbakov, A. Pöthig, A. Kartouzian, I. D. Sharp, C. Katan, J. Even, F. Deschler, *Sci. Adv.* **2023**, *9*, eadh5083 HAL

[3] M. Kepenekian, J. Even, *J. Phys. Chem. Lett.* **2017**, *8*, 3362 HAL

Profile of the candidate | A Master degree in Chemistry, Materials Sciences, Physics or related disciplines is required. A strong background in any of the following subject is desired: quantum chemistry, solid-state physics, materials modelling approaches, and atomistic simulations. The successful candidate should be highly motivated, with excellent communication skills and the ability to work in close collaboration with experimentalists and other theoreticians.

The CTI team | The postdoctoral researcher will work in the Theoretical Inorganic Chemistry (*Chimie Théorique Inorganique*, CTI) team at the Institut des Sciences Chimiques de Rennes (ISCR). The CTI team gathers computational chemists and physicists (15 permanent staff members, 15 students) with complementary skills, working with a broad set of quantum chemical tools, ranging from high precision ab initio wave function-based calculations to fast semi-empirical methods. CTI team members are interested in diverse type of systems, including isolated species, bulk materials and surfaces, mainly of high experimental and societal interest. The CTI team thus provides a stimulating scientific environment, also offering regular team meetings, invited seminars as well as visitors internationally recognized. Considerable local, national and European computing resources are available for the purposes of the scientific projects.



How to apply | Candidates should apply via the CNRS plateforme (reference UMR6226-MIKKEP-003) and join to their application an up-to-date CV and a motivation letter.