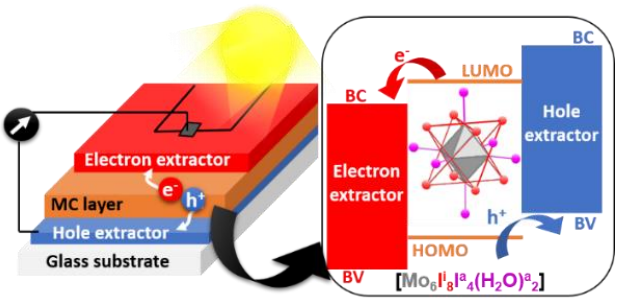
Ph.D project 2023-2026

Nano-building blocks based on octahedraL molybdenum clusters for the design of structured inorganic photoelectrodes for solar energy conversion

Rennes Institute of Chemical Sciences (UMR CNRS 6226) – Univ. Rennes

Required skills:
- Master 2 course
- Motivation for experimental chemistry and chemical physics (synthesis and characterization of materials)
- Mastering English
- Ability to work in a team, good organization, good communication skills (written and oral)
- Requested documents: CV, results of M1 or equivalent level, M1 (or L3 or equivalent levels) internship report, for an interview

Description:



Scientific Context. In the context of the global warming, the need to develop low-carbon, clean, inexpensive and reliable energies motivates research efforts to design efficient and clean solar energy conversion systems. The thesis subject is part of the ANR project NanoLEtsGOs that aims to develop new light-collecting layers (photoelectrodes), free of strategic and/or toxic elements, which can be integrated into photovoltaic cells. The project focuses on the design of photoelectrodes based on molecular inorganic nano-objects, the octahedral Molybdenum clusters (MC), composed of Mo, one of the main low-toxic industrial metals. MC halides (Mo_6X_{14}, X = Cl, Br, I) have remarkable optical and electronic characteristics (strong absorption in the visible, lifetime in the 1-1000 µs range, ambipolar properties) necessary for their use as a collector of light in efficient solar cells.[1-7] The NanoLEtsGOS project aims to optimize the optical and electronic properties (collection of light, separation and transport of charges) of the MC-based layers *via* the control of the interactions between these nano-objects. The thesis will focus on the controlled assembly of these molecular building blocks according to two strategies: i) the progressive condensation of the MCs and ii) the incorporation into a conductive polymer matrix.

Topic. The thesis work revolves around two axes corresponding to the two assembly strategies of MCs. The control of the degree of condensation of MCs will be explored *via* solution chemistry pathways through the progressive substitution of halogen ligands by sulfur. The incorporation into a polymer matrix using electrostatic or supramolecular approaches is an axis already developed at the ISCR.[6,7] The synthesis of polymers will not be the subject of the thesis. These will be synthesized on demand within the framework of the ANR project. The student will focus more specifically on the integration of MCs and on the deposition of layers. The optical and electronic properties of the photoelectrodes obtained after deposition of the cluster layers will be studied by combining optical (UV-vis, photoluminescence), electrochemical (photoelectrochemistry, complex impedance) and spectroscopic (XPS, UPS) characterization techniques. The dynamics of charge transfer and the construction of the energy diagrams of the photoelectrodes will make it possible, on the one hand, to estimate the potential of such photoactive layers, and on the other hand, to select the charge extractor electrode materials for the design of solar cells. The realization and the study of the performances of the latter will be carried out during the last year of the thesis work.

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ISCR contacts:

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References

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[2] A. Renaud et al., Electrochimica Acta 2019, 317, 737.
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[4] Y. Zhao et al., Adv. Energy Mater. 2013, 3, 1143.
[5] K. Costuas et al., Phys. Chem. Chem. Phys. 2015, 17, 28574.
[6] M. Amela-Cortes et al., J. Mater. Chem. C 2014, 2, 1545.
[7] S. Khlifi et al., J. Mater. Chem. C 2021, 9, 7094.