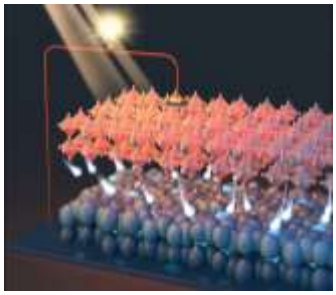
Internship proposal:

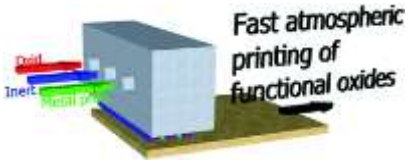
Fabrication of NiO films for perovskite solar cells

Summary: Halide perovskite solar cells (PSCs) have attracted a lot of attention due their high performance and low cost. Up to now, the highest device efficiencies were achieved by employing n-type SnO_2 and TiO_2 electrodes. However, the comparably large high temperature process required in mesoporous TiO_2 structures severely limits the further commercial application. Inverted PSCs (*p-i-n* structure) using p-type NiO as the hole transport layer (HTL) have attracted massive attention in recent years due to their lower processing temperature for large scale and flexible devices, negligible hysteresis effects, and furthermore, better stability as compared to organic HTLs.[1] However, the reported efficiencies of inverted PSCs are still lower than that of conventional PSCs due to the low conductivity and a mismatched band position of NiO.



The properties of nickel oxide films can be tuned using several strategies, such as deposition method, doping, and surface functionalization. The goal of the internship is to fabricate NiO films as HTLs with optimal properties for the PSCs. The student will fabricate and systematically study the films using various methods:

- Sol—gel processing is based on the deposition NiO films from the solution of the various Ni precursors[2]
- Nanoparticle coating will rely first on the synthesis of NiO nanocrystals followed by their deposition and annealing.
- Spatial atomic layer deposition (SALD) will be performed using a state-of- the-art reactor from LMGP lab. This technique allows depositing nanoscale layers at low cost and high rate and can be adapted to obtain the thickness or composition gradients.[3]



After mastering the deposition of the films by the three techniques, we will then carry out doping of the NiO films with various ions, which will be an effective way to adjust the electrical and optical properties of the films.[4] In addition, we will systematically study surface functionalization using different functional molecules and its influence on the properties of the NiO and solar stacks.

The student will carry out the NiO deposition using various state-of -the-art techniques controlling the composition and morphology. He/she will study the properties of the films using optical spectroscopies, AFM, XRD and other techniques. The internship will take place at the SyMMES (CEA Grenoble) and LMGP labs, who are experts in the NiO deposition using different techniques collaborating closely with a PhD student working on a similar topic. The films will be then further studied and tested for the solar cells at the IPVF institute in Palaiseau.

Related Publications

(1) Aumaitre, C.; Joly, D.; Aldakov, D.; Demadrille, R. in *The Future of Semiconductor Oxides in Next-Generation Solar Cells*; Elsevier, 2018; pp 85–115.
(2) Li, Y.; Ye, J.-J.; Medjahed, A.; Aldakov, D.; Pouget, S.; Djurado, E.; Xu, L.; Reiss, P. *ACS Appl. Energy Mater.* **2023**, *6* (3), 1555–1564.
(3) R. L. Z. Hoye, D. Muñoz-Rojas, Z. Sun, H. Okcu, H. Asgarimoghaddam, J. L. MacManus-Driscoll, K. P. Musselman *PRX Energy, 2025, 4, 017002*
(4) Ye, J.; Li, Y.; Medjahed, A. A.; Pouget, S.; Aldakov, D.; Liu, Y.; Reiss, P. *Small* **2021**, *17* (5), 2005671.

Background and skills expected

Chemistry or Chemistry of materials, nano/organic chemistry, knowledge of deposition techniques

Competences that will be acquired during the internship

Deposition of semiconductor films using various cutting-edge methods; characterization of the thin films using modern equipment (XRD, AFM…); work in the collaborative environment with the experts in the field, such as IPVF

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Laboratories: CEA-Grenoble/SyMMES (Synthesis, Properties and Structure of Functional Materials), LMGP (Laboratory of Materials and Engineering)

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