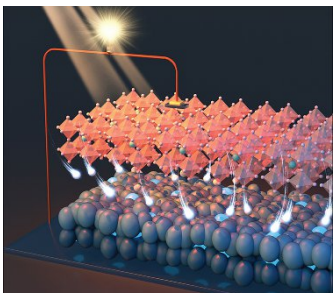
Master thesis proposal

Fabrication of NiO films for perovskite solar cells

Keywords : photovoltaics, thin films, NiO, hybrid perovskites, combinatorial deposition, spatial atomic layer deposition, PEPR DIADEME FASTANANO, PEPR TASE IOTA

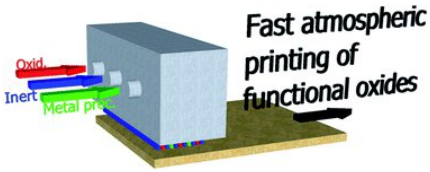
SCIENTIFIC DESCRIPTION :



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:

- The combinatorial Spatial atomic layer deposition (SALD) platform at 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]
- Film surface engineering by deposition of different functional molecules will be performed in collaboration wuth SyMMES, to evaluate the properties onf the NiO and solar stacks.



Doping of the NiO films with various ions, which will be an effective way to adjust the electrical and optical properties of the films,[3] will be explored.

The student will study the properties of the films using optical spectroscopies, AFM, XRD and other techniques. The internship will take place at LMGP and the SyMMES (CEA Grenoble), 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.

REFS:

(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) 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*
(3) Ye, J.; Li, Y.; Medjahed, A. A.; Pouget, S.; Aldakov, D.; Liu, Y.; Reiss, P. *Small* **2021**, *17* (5), 2005671

Techniques/methods in use : combinatorial SALD

Master thesis proposal

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

Industrial partnership : David Muñoz-Rojas, LMGP, in collaboration with SyMMES and IPVF. Intercollabration between PEPR DIADEME and TASE

Internship supervisor(s) : David MUÑOZ-ROJAS, david.munoz-rojas@grenoble-inp.fr, 0687960790

Internship location : Grenoble (LMGP,Symmes)