SORBONNE UNIVERSITÉ

# Sorbonne Université/ China Scholarship Council program 2020

## Thesis proposal

Title of the research project: Rational design of solar cells based on lead halide perovskite nanocrystals and 2D materials

Keywords: lead halide perovskite nanocrystals, 2D materials, electronic structure

Joint supervision: ~~yes (name/surname)~~ /no

Joint PhD (cotutelle): ~~yes (name/surname)~~ /no


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Institution: Sorbonne Université

Doctoral school (N°+name): ED397 Physique et Chimie des Matériaux ………………………………………..

Research laboratory: Institut des Nanosciences de Paris

Address of the laboratory: 4 place Jussieu, BC840, 75005 Paris………………..…………………………………………

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## Subject description (2 pages max):

### 1) Study context

Defect tolerant nanocrystals (NCs) representing lead halide perovskite lattice have recently demonstrated to display remarkable photoluminescence (PL) efficiency up to 90% while offering notable colour purity in comparison with that of organic dye molecules [Protesescu2015]. Moreover the optical band gap of these new perovskites NCs (PeNCs) can be simply tuned by changing their composition offering a large range of colour emitters or absorbers covering the entire visible spectrum from red to violet. Owing to their exceptional optical properties PeNCs are promising candidates for highly efficient photovoltaic devices using PeNCs with optical gap covering the sun spectrum in a simple design.

The power conversion efficiency of solar depends not only on the light harvesting material (absorbent) but also on the ability of transport layers to extract charges effectively. In this context, the optimization of a solar cell device strongly depends on both: the intrinsic nanocrystal opto-electronic properties and their interaction with the transport layers. While the proof of concept for solar cells based on PeNCs was demonstrated recently [Swankar2016], the goal of the present project is to explore the design of PeNCs based solar cell in conjugation with 2D materials as charge carrier layers, employing solution processing. Further, our approach will rationalize the design by building a comprehensive understanding of the PeNCs electronic structure, interface interaction and by unravelling the interplay with radiation / temperature / moisture that affects the performances of the device. The ultimate objective of the project will be to demonstrate the feasibility of cost effective solar cells with PeNCs and 2D materials.

Expected objectives and results include:

1. Generating new fundamental knowledge of underlying mechanisms for functional materials in a highly efficient solar energy conversion devices
2. Characterizing electronic structure and energy band alignment of high performance solution processed 2D materials (Xene, dichalcogenide) and PeNCs
3. Limiting non-radiative recombination losses by elucidating interface interaction of PeNCs at dichalcogenide interface on model systems
4. Designing a rationalized architecture incorporating PeNCs and 2D materials for hole transport (HTL) and electron transport (ETL)
5. Characterization of the optimized architecture

## 2) Details of the proposal

During the first year, the PhD candidate will be trained during three months to vacuum technologies and electron spectroscopies available in the lab. The PhD candidate will then characterize the electronic properties of the 2D materials produced by collaborators in Dresden (Pr. Xinliang Feng) [Zhang2019] and PeNC synthetized in Paris and compare the influence of deposition methods (spin coating, spray). The PhD will work on the determination of majory/minority carrier in PeNC using electron spectroscopies related techniques [Amelot2020]. During the second year, the interplay between 2D materials and PeNC will be investigated by means of electron spectroscopies firstly on model systems (2D materials single crystals), next on real systems using 2D inks. The stability of 2D materials and PeNC will be also investigated. During the third and fourth year, the PhD candidate will work on the design of solar cell architecture based on PeNC and 2D materials in collaboration with BCMaterials in Bilbao to characterize figure of merit of devices [Ahmad2018]. Mobility periods at BCMaterials can be foreseen within the project.

### 3) References (bold from the team and collaborators)

[Protesescu2015] L. Protesescu, et al., Nano Lett. 15, 3692-3696 (2015) DOI: 10.1021/nl5048779
[Swankar2016] A. Swankar, et al., Science 354, 92–95 (2016) DOI: 10.1126/science.aag2700
**[Zhang2019] P. Zhang et al., Small 2019, 15, 1901265 DOI : 10.1002/smll.201901265**
**[Amelot2020] D. Amelot, et al , J. Phys. Chem. C (2020), 124, 6, 3873-3880 https://doi.org/10.1021/acs.jpcc.9b10946**
**[Ahmad2018] S.Ahmad, et.al., Nano Energy 50 , 220–228 (2018) DOI:10.1016/j.nanoen.2018.05.035**

### 4°) Profile of the Applicant (skills/diploma…)

The recruited PhD candidate will hold a master or equivalent in solid state physics, material physics, nanophysics or equivalent with a strong background in condensed matter physics. Knowledge of deposition techniques by spin coating/and/or vacuum depositions will be appreciated. Female applicants are encouraged to apply.

## Contacts:

### Thesis supervisor

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