POLITECNICO MILANO 1863

Supervisor Expression of Interest
MSCA - Marie Sklodowska Curie Action - (PF) Postdoctoral Fellowship 2023

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Department Name: Chemistry, Materials and Chemical Engineering "G. Natta" (CMIC)

Research topic:

- □MSCA-PF Research Area Panels:
- □CHE_Chemistry
- □ECO_Economic Sciences
- □ENG_Information Science and Engineering
- □ENV_Environmental and Geosciences
- □LIF_Life Sciences
- □MAT_Mathematics
- □PHY_Physics
- □SOC_Social Sciences and Humanities

Brief description of the Department and Research Group (including URL if applicable):

The project will be based at the Department of Chemistry, Materials and Chemical Engineering "Giulio Natta" (CMIC, https://www.cmic.polimi.it/en/) of Politecnico di Milano, and Laboratory of Supramolecular and Bio-Nanomaterials (https://www.suprabionano.eu/). The Department offers chemical lab facilities and instrumentations such NMR facilities, XRD facilities and microscopy facilities with all the necessary equipment to conduct relevant analyses foreseen in the project. Specifically, the SBNLab possesses unique expertise in organic synthesis and fluorine chemistry, in the characterization of fluorinated and polyhalogenated materials, as well as in crystal engineering, molecular recognition, and supramolecular chemistry, with state-of-the-art instrumentation for crystal structure determination.

TITLE of the project:
Lead-Free hybrid Organic-inoRganic pErovskites FoR OptoelectroNic applicaTions (FOREFRONT)

Brief project description:

In the last decade, **hybrid organic-inorganic perovskites (HOIPs)** have emerged as a flourishing area of research.[1] Their ease and low-cost production together with their unique optoelectronic properties make them promising semiconducting materials, for a multitude of applications. In particular, HOIPs hold great potential for the next generation solar cells and great progress has been made in this field reaching conversion efficiency higher than 25% in few years.[2] However, toxicity issues related to lead-based halide perovskites together with their poor stability in air and moisture, still hinder their practical implementation in optoelectronic devices. In this scenario there is an urgent need **to develop benign and stable lead-free perovskites** with tunable optoelectronic properties.
Tin or germanium are considered the best options to replace lead, however Sn and Ge-based perovskites are highly sensitive to oxygen and moisture, being easily decomposed by oxidation.[3] Bi, Sb, or Cu-based perovskites are more stable, however their efficiency is very low[4] and further optimization of their bandgaps, charge transporting properties as well as film morphology are highly needed in order to develop efficient optoelectronic materials.
It is generally accepted that the presence of defects, both at the surface or in the bulk, is critical for the long-term stability and considerably limits perovskite efficiency.[5] Therefore, optimizing chemical composition of materials and **exploiting non-covalent interactions** for interfacial engineering, defects engineering, and defect passivation are efficient routes towards enhancing the overall efficiency and stability of PSCs.[6]
In this context, some key-aspects to be possibly considered and addressed via a specific project proposal are, among others:

1) Application of **highly hydrophobic additives** for moisture-resistant lead-free HOIPs with improved surface morphology and grain boundary;
2) Application of **new passivating agents**, specifically designed to trap under-coordinated halide anions and prevent charge recombination onto perovskite surface;
3) Development of **new organic cations** for the obtainment of low dimensional (2D, quasi-2D, 1D or 0D) lead-free HOIPs with improved stability and enhanced optical properties.

Finally, understanding the structure-property relationship, as well as the assessment of the optical, electronic and optoelectronic properties of such materials is a fundamental issue.

References

1) Y. Zhao, K. Zhu *Chem. Soc. Rev.*, **2016**,*45*, 655
2) M. A. Green, E.D. Dunlop, J. Hohl-Ebinger, M. Yoshita, N. Kopidakis, A.W.Y. Ho-Baillie *Prog Photovolt Res Appl.* **2020**;*28*,3
3) W. Ke, M.G. Kanatzidis Nat Commun **2019**, *10*, 965
4) Y. Gao, Y. Pan, F. Zhou, G. Niu, C. Yan *J. Mater. Chem. A*, **2021**, *9*, 11931
5) F. Wang, S. Bai, W.Tress, A. Hagfeldt, F. Gao1. *npj Flex Electron* **2018**, *2*, 22
6) P. Metrangolo, L. Canil, A. Abate,* G. Terraneo, G. Cavallo Angew. Chem. Int. Ed. 2022, e202114793