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Supervisor Expression of Interest
MSCA - Marie Sklodowska Curie Action - (PF) Postdoctoral Fellowship 2021

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Department Name:	Chemistry, Materials and Chemical Engineering "G. Natta" (DCMC)
Research topic: (https://www.polimi.it/en/scientific-research/research-at-the-politecnico/departments/)	**Intermolecular and Surface Interactions in Engineering Perovskite Solar Cell Materials (Engineer-PSC)** PE5_16 Supramolecular chemistry PE5_1 Structural properties of materials
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
Politecnico di Milano Areas:	☐ Cultural Heritage ☐ Smart Cities ☐ Horizon Europe Missions ☐ Health ☐ Industry 4.0

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Title and 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 facility, XRD facility 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.

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Brief project description: (max 1 page)	**Intermolecular and Surface Interactions in Engineering Perovskite Solar Cell Materials (Engineer-PSC)** In the last decade, **organic-inorganic hybrid halide perovskites** (OIHPs) 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, OIHPs 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, the practical implementation of perovskite solar cells (PSCs) is still hindered by their poor stability in air and moisture, which is responsible for their short lifetime. 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 device efficiency.[3] 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.[4] In this context, some key-aspects to be possibly considered and addressed via a specific project proposal are, among others: 1) Application of **new passivating agents**, specifically designed to trap under-coordinated halide anions and prevent charge recombination onto perovskite surface; 2) Design of new **organic interfacial modifiers** able to improve the contact between perovskite and electron transporting layers for an efficient charge transfer; 3) Application of **highly hydrophobic additives** for moisture-resistant perovskites with improved surface morphology and grain boundary; 4) Development of **new organic cations** for the obtainment of low dimensional (2D, quasi-2D and 1D) perovskites with improved stability and enhanced optical properties. Finally, understanding the structure-property relationship, as well as the assessment of the optical, electronic, optoelectronic properties of such materials is a fundamental issue. 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) F. Wang, S. Bai, W.Tress, A. Hagfeldt, F. Gao1. *npj Flex Electron* **2018**, *2*, 22 4) M. Zhu, C. Li, B. Li, J. Zhang, Y. Sun, W. Guo, Z. Zhou, S. Pang, Y. Yan *Mater. Horiz.*, **2020**,*7*, 2208