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Supervisor Expression of Interest
MSCA-IF Marie Sklodowska Curie Action-Individual Fellowship 2020

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Department Name: Research topic: (https://www.polimi.it/en/scientific-research/research-at-the-politecnico/departments/)	Chemistry, Materials and Chemical Engineering (DCMC) PE4_13 Theoretical and computational chemistry PE3_4 Electronic properties of materials, surfaces, interfaces, nanostructures, etc.
MSCA-IF Research Area Panels	☐ CHE_Chemistry ☐ PHY_Physics
Politecnico di Milano Areas:	☐ Industry 4.0
Brief description of the Department and Research Group (including URL if applicable):	DCMC is large Department combining expertise in chemistry and materials spanning over ten order of magnitude in length, from the molecular scale to that of chemical plants or buildings: https://www.cmic.polimi.it/en/ Research will be carried out within the Materials Modelling, Morphology & Structure Lab (^{3}MoSt) of DCMC: https://3most.chem.polimi.it/ (under construction). The ^{3}Most personnel currently consists of three full professors, three associate professors and one research associate (RTDB), as well as several PhD and postdoctoral associates. Research in the Raos group focuses on the theoretical modelling—from electronic structure up to coarse-grained molecular dynamics—of pi-conjugated materials, polymers and polymer networks, nanocomposites, and soft matter in general: https://scholar.google.com/citations?hl=it&user=NmoHoYYAAAAJ Experimental groups within the ^{3}Most lab carry our structural and morphological studies of materials by X-ray scattering and electron microscopies. The group also collaborates with other experimental groups in the Department (e.g., NMR of soft matter) and elsewhere. In recent years the group has attracted about 1M€ in competitive (PRIN, Fondazione Cariplo) and industrial funding (Eni, Pirelli Tyre, Aditya Birla, etc.).

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Brief project description: (max 1 page)	**Charge separation in organic photovoltaics: quantum mechanics at the mesoscale.** Harnessing of sunlight by photovoltaics plays an important role within any realistic, sustainable energy scenario.[1] Several alternatives are competing to replace silicon as the next-generation technology. Recently, there has been a resurgence of interest in organic photovoltaics (OPV),[2] thanks to their environmental friendliness, low cost, printability on flexible substrates, chemical tunability. Considerable progress has been made in the production of high performing OPV cells (>12% power conversion efficiencies), through the synthesis of better donor (D) and acceptor (A) molecules and polymers, optimization of their morphology within the active layer of the OPV films, improvement in charge extraction efficiency at the electrodes, etc.[3] The mechanisms of the primary event of charge separation—production of an electron-hole pair at a D/A interface, following absorption of a photon within the OPV film—remain elusive. Different theoretical models can be used to gain an understanding of the experimental data, such as current-voltage curves and time-resolved spectroscopies.[4] The so-called mesoscale (10^1 nm), which characterizes the morphology of good "bulk heterojunction" cells, is critical for charge separation. Quantum mechanical coherence phenomena appear to be at work,[5] but for different reasons they cannot be modeled effectively by any of the standard methods (e.g., quantum chemistry at the molecular scale or kinetic Monte Carlo at the device scale). Our group has proposed a coarse-grained quantum chemical method, explicitly designed to deal with coherent charge separation phenomena at the mesoscale.[6] Each D or A molecule is modelled as one site carrying two electrons within two orbitals (HOMO and LUMO). The model can be parametrized on specific systems and allows the calculation of electronic states on assemblies of thousands of D and A molecules, including electrostatic effects (electron-hole interactions). Calculation on such model systems have already demonstrated that delocalization of the electrons and holes over tens of sites can effectively reduce their binding energies to a few times k_BT, compatible with the near-100% efficiency of charge separation observed in the best devices.[7] We are seeking a brilliant, highly motivated post-doctoral associate who will extend the method and apply it to realistic models of D/A interfaces, such as those which can be produced by molecular dynamics simulations. Experience with programming and interest in method development are important prerequisites for this position. (1) S. Chu et al. The Path towards Sustainable Energy. *Nat. Mater.* **2017**, *16*, 16. (2) Li, G.; Zhu, R.; Yang, Y. Polymer Solar Cells. *Nat. Photonics* **2012**, *6*, 153. (3) J. Zhao et al., Efficient Organic Solar Cells Processed from Hydrocarbon Solvents. *Nat. Energy* **2016**, 1, 15027. (4) S. Few, J. Frost, J. Nelson, Models of Charge Pair Generation in Organic Solar Cells. *Phys. Chem. Chem. Phys.* **2015**, 17, 2311. (5) J.L. Brédas, E.A. Sargent, G.D. Scholes, Photovoltaic Concepts Inspired by Coherence Effects in Photosynthetic Systems. *Nat. Mater.* **2017**, *16*, 35. (6) G. Raos, M. Casalegno, J. Idé, An Effective Two-Orbital Quantum Chemical Model for Organic Photovoltaic Materials. *J. Chem. Theory Comput.* **2014**, *10*, 364. (7) M. Casalegno et al., Origin of Charge Separation at OPV Heterojunctions: A Mesoscale Quantum Mechanical View. *J. Phys. Chem. C* **2017**, 121, 16693.