

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

Supervisor name: Carlo S. Casari

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Research topic:

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

Brief description of the Department and Research Group:

The activity will be carried out in a research environment characterized by a high level of expertise and outstanding results. The Micro and Nanostructured Materials Laboratory - NanoLab of the Department of Energy is focused on the experimental development and understanding of novel materials. NanoLab hosts or hosted a total of six ERC projects (two ERC Consolidator grants and four Proof-of-Concept ERC grants), one EIC Transition project, and two MSCA grantees. Nanolab is composed of 8 academic staff, 10 postdocs, more than 15 PhD students, and 20 master students with state-of-the-art experimental facilities in 500 m² of laboratories.

The Department of Energy (www.energia.polimi.it) has a total staff exceeding 350 people working in experimental and modelling and numerical simulation laboratories on a total area of more than 10,000 m². Sophisticated and advanced equipment allows excellent performance, alongside prestigious Companies and with authoritative research centres in Italy and in the world. The Department of Energy has been awarded by the Italian Ministry of Education, University and Research (MIUR) as "Department of Excellence" in 2018.

Prof. Carlo S. Casari is an ERC consolidator grantee (ERC-2016-CoG, see www.esplore.polimi.it), he got 2 Proof of Concept grants in 2019 and 2022 and he is coordinating a EIC Transition project. He won innovation prizes including Switch2Product by PoliHub, Startcup Lombardia and Italian National Innovation Prize PNI and in 2023 he founded the startup (and spinoff of POLIMI) ENIGMA srl.

www.energia.polimi.it www.esplore.polimi.it



TITLE of the project: Development of novel materials based on sp-carbon linear nanostructures from fundamental science to applications

Brief project description:

In the last 30 years, the discovery of fullerenes, nanotubes, and graphene has nurtured the interest in linear carbon structures with *sp*-hybridization in the form of carbon atomic wires. Carbon-atom wires represent the ultimate 1-D carbon system (i.e. carbyne) and are interesting for fundamental and applied science. Recent theoretical calculations have outlined outstanding mechanical, thermal, and electronic properties which can be tuned by controlling the wire length and the terminating functional group.

The design and control of the wire structure open the way to building materials with tunable properties, which is at present a largely unexplored topic. The activity is in the framework of the project *EspLORE* (www.esplore.polimi.it) funded by the European Research Council (ERC Consolidator grant). The core concept of *EspLORE* is to exploit the present fundamental knowledge of carbon-atom wires as isolated molecules/nanostructures to explore the applied science and engineering of new materials in the form of thin film assemblies and nanocomposites, so to fill the large existing gap between basic science and engineering.

The proposed methodology includes fabrication of sp-carbon atomic wires by physical methods, their deposition/assembling on surfaces, and the experimental study of structural, electronic and optical properties (supported by density functional theory calculations) in view of potential application in optolectronics and energy storage. Structure-property relationship is investigated at a multiscale level, moving from the single wire level (atomic scale) to multi-wire interactions (nanoscale) and up to extended systems (macroscale).

The research activity is focused on the experimental fabrication and investigation of sp-carbon atomic wires (linear sp-hybridized carbon nanostructures) and on the development of wire-based materials. The characterization is done mainly by vibrational spectroscopy (Raman, SERS). The assessment of the functional properties as well as the understanding of the structure-property relationship is a fundamental issue.