POLITECNICO
MILANO 1863

Supervisor Expression of Interest
MSCA - Marie Sklodowska Curie Action - (PF) Postdoctoral Fellowship 2024

Supervisor name: Piero Macchi

Email address: piero.macchi@polimi.it
Link "Pagina docente": https://3most.chem.polimi.it/pieromacchi/
Department Name: Chemistry, Materials and Chemical Engineering

Research topic: Spintronics materials

MSCA-PF Research Area Panels:

- ☐ECO_Economic Sciences
- ☐ENG_Information Science and Engineering
- ☐ENV_Environmental and Geosciences
- ☐LIF_Life Sciences
- ☐MAT_Mathematics
- ☐PHY_Physics
- ☐SOC_Social Sciences and Humanities
- X CHE_Chemistry

Brief description of the Department and Research Group (including URL if applicable):
Department of Chemistry, Materials, and Chemical Engineering.
https://www.cmic.polimi.it/
The department has a distinctive multi-discipline nature, from the aggregation of researchers active in these disciplines. More than 150 faculty members are actively teaching and researching. The research topics of the Department's activity and scientific production fall within these general areas:
- Biomedical Engineering
- Construction, Durability and Cultural Heritage
- Materials Engineering & Nanotechnology
- Molecular Sciences
- Process Engineering & Manufacturing
- Renewable Materials and Circular Economy

The department is equipped with many research laboratories, including three department laboratories and several inter-department laboratories, for analysis and characterization of the materials, which is a vital step for the discovery and the development of new materials.

Laboratory of Materials Modelling, Morphology and Structure (^{3}MoStLab)
https://3most.chem.polimi.it/

The central endeavor in this laboratory is identifying and detailing key structure-property relationships in molecular or polymeric materials. We exploit experimental techniques and theoretical modelling to characterize the structure and the properties of crystalline, semicrystalline or amorphous, organic, inorganic, metal-organic and hybrid materials. Prof. Macchi is interested in metal-organic frameworks for applications in electronics, spintronics, sustainable energy production and storage.
The experimental techniques are mainly based on X-ray diffraction (in home laboratories or at large scale facilities) and neutrons diffraction at large scale facilities, for example at the Paul Scherrer Institute, in Villigen (CH). Spectroscopic and calorimetric techniques, such as impedance spectroscopy and differential scanning calorimetry, are also employed. These enable investigating the dynamics and morphologies of the samples. The theoretical modelling is carried out using ab initio molecular quantum mechanics and quantum crystallographic methods.

TITLE of the project:
New disruptive coordination network materials for spintronic applications

Brief project description:

Scope. The rapid development of quantum information processing has an unprecedented impact on communication technologies, but also produced an increasing demand of new, high performing materials. In the recent years, together with the improvement of metallic and ceramic materials for spintronic applications, new directions have emerged using organometallic coordination networks that, just like their inorganic counterparts, are able to generate topological materials and ferro- or antiferromagnetic lattices. In addition, the opportunity offered by coordination networks stands in the unmatchable flexibility of these species, both in terms of composition and structural motifs. While the compositional freedom can be exploited in the design and fabrication of these materials, the structural flexibility may also depend on the applications of external stimuli, such as pressure, temperature gradient, electric or magnetic field.
The research group of prof. Piero Macchi has intensively investigated a number of coordination networks obtained from the self assembly of magnetic metal ions (such as Cu^{2+}, Ni^{2+}, Co^{2+}, etc.) and some organic linkers (for example aromatic aza-heterocycles, multidentate anions of carboxylic acids), used as carriers of the spin state information. For these materials, the experimental and theoretical charge density distribution and the magnetization have been investigated, including changes induced by the application of mechanical pressure. The organic linkers tested so far have not optimized their capacity to transfer the spin state information, especially because of stereo-electronic reasons. However, more recent studies addressed materials based on formate as the most promising anti-ferromagnetic networks within the class of coordination polymers. This has enabled stating new criteria for the selection of optimal linkers, based on the classical Goodenough-Kanamori-Anderson (GKA) rules valid for traditional metal oxides.

Research hypothesis. The hypothesis of this project is: we can find rules that are more appropriate for the linkers featuring peculiarities like multiple hapticity (different coordination modes) and atoms with double kind of coordination ability to a metal (like σ and π electrons, bonding and back-bonding ability, etc.), going beyond GKA rules and their extension to coordination networks.

POLITECNICO
MILANO 1863

Research plan. In order to test the main hypothesis of this research project, the following plan will be adopted: a) selecting classes of linkers known to produce bidimensional or tridimensional networks in combination with magnetic metal ions; b) preparing the compounds (known from the literature or synthesized for the first time, for those linkers for which a proper network is not yet known); investigating experimentally and theoretically the charge density distribution; d) investigating experimentally and theoretically the magnetic susceptibility and modelling the magnetic network; e) test changes to the magnetic network induced by external stimuli; f) rationalizing the results and draw new criteria for the choice of optimal linkers.

Methods. The research plan requires: a) preparations of the materials (with in air or solvothermal synthesis); b) structural characterization with X-ray diffraction (including high resolution for the charge density determination); c) superconducting quantum interference (squid) measurement or muon spectroscopy for the measurement of the magnetic susceptibility; d) neutron diffraction experiments for the determination of the magnetic structures; e) high pressure X-ray diffraction and magnetization measurements; f) density functional theory calculations for the prediction of the structural and magnetic properties. Point a-b and e-f can be carried out within the laboratory of the department facilities. Neutron diffraction experiments can be carried out at large scale facilities (like sinQ at PSI, ILL, and ISIS). The SQUID or the muon spectroscopy can be obtained in cooperation with external colleagues.

Expected results. We expect to successfully extrapolate new rules for the selection of optimal linkers for the preparation of more efficient, tuneable, and multifunctional new materials for spintronic.