One Postdoc position is available at the Department of Chemistry and Industrial Chemistry of the University of Genova, Italy.

**Topic:** Study of intermetallic catalysts for the $CO_2$ methanation

**Faculty Sponsor**: Riccardo Freccero (riccardo.freccero@unige.it)

**Description:** Intermetallic compounds (IMC) are a large family of inorganic materials featuring complex crystalline and electronic structures. Consequently, the study of their chemical properties, such as reactivity, has often been overlooked in comparison to that of their physical properties. The development of new theories that describe their chemical bonding has recently increased their appeal as heterogeneous catalysts. The reduction of $CO_2$ to $CH_4$ by means of IMC constitutes a new research field. The project aims to synthesize multi-component IMC free of the noble metals commonly used in the methanation reaction, such as ruthenium, able to form IM hydrides active in the Sabatier reaction ($CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O$). The characterization will be performed by electron microscopy (FE-SEM and TEM) and X-ray diffraction both on powders and single crystals. Aiming at understanding the main factors determining the activity of a given IMC, DFT-based quantum chemical calculations and surface simulations will be performed by employing chemical bonding analysis methods in position-space, in particular the Quantum Theory of Atoms in Molecules (QTAIM) and the Electron Localizability Indicator (ELI-D).

**Application** is available at the following link: https://unige.it/en/concorsi/calls-research-grants (Call 1936 of 27.4.2023 - RESEARCH PROGRAM NO. 6)

**Deadline:** 29/05/2023 12.00 pm CET

**Start date:** September 1, 2023 (01/09/2023)

**Postdoc Appointment Term**: One year

**Location:** candidate will be based at the Department of Chemistry and Industrial Chemistry of the University of Genova, Italy.