Chiral "doped" MOFs: an electrochemical and theoretical integrated study

Rufaro Kawondera, Marco Bonechi, Irene Maccioni, Walter Giurlani, Tommaso Salzillo, Elisabetta Venuti, Debabrata Mishra, Claudio Fontanesi, Massimo Innocenti, Gift Mehlana and Wilbert Mtangi

Abstract

This work reports on the electrochemical behaviour of Fe and Zn based metal-organic framework (MOF) compounds, which are "doped" with chiral molecules, namely: cysteine and camphor sulfonic acid. Their electrochemical behaviour was thoroughly investigated via "solid-state" electrochemical measurements, exploiting an "ad hoc" tailored experimental set-up: a paste obtained by carefully mixing the MOF with graphite powder is deposited on a glassy carbon (GC) surface. The latter serves as the working electrode (WE) in cyclic voltammetry (CV) measurements. Infrared (IR), X-ray diffraction (XRD) and absorbance (UV-Vis) techniques are exploited for a further characterization of the MOFs' structural and electronic properties. The experimental results are then compared with DFT based quantum mechanical calculations. The electronic and structural properties of the MOFs synthesized in this study depend mainly on the type of metal center, and to a minor extent on the chemical nature of the dopant.

Keywords: SEM; XRD; chiral doping; cyclic voltammetry; metal-organic framework; solid state electrochemistry.