PhD Proposal 2017

School: CentraleSupelec	
Laboratory: SPMS	**Web site: www.spms.ecp.fr**
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Title: Charge density studies on functionalized polyoxomolybdate of potent biological properties
Scientific field: Chemistry, crystallography
Key words: polyoxometallate, charge density, electrostatic potential

Details for the subject:

Background, Context:

Among the reported nanoscale polyoxometallate POMs, [1] some POMs have been discovered to show remarkable self-assembly in solution [2] or on surfaces, [3] and even to function as artificial cells to model the transport of cations under physiological conditions [4]. Polyoxovanadate (POV) is a class of compound with various properties in chemistry, magnetism and pharmaceutical chemistry [5]. Charge density studies on vanadium compounds are rare [6]. Our group (SPMS, UMR 8580, Ecole Centrale Paris) has already performed such a study on the two different decavanadate co-crystals [7], and two functionalized hexavanadate [8] (figure 1) leading to the determination of the experimental electrostatic potential for the two compounds, as well as topology analysis and determination of the *d* orbital population of the vanadium atom. The *ab initio* charge density studies for these compounds have also been determined.

The group of Pr. Yongge Wei (Department of Chemistry, University of Tsinghua, Beijing) has extensively worked on the chemistry of functionalized polyoxomolybdate [9].

The aim of the PhD is to perform charge density studies on new polyoxomolybdate synthesized at the Department of Chemistry of Tsinghua.

Research subject, work plan:

Synthesis will be carried out at Tsinghua University. Crystallization and molecular structure will be done at CentraleSupelec (laboratoire SPMS) on new functionalized polymolybdate. On suitable crystals, high resolution X-ray diffraction will be performed in order to determine electron and electrostatic properties. The experiments will be done at the diffraction center of SPMS or using the synchrotron radiation at SOLEIL. *Ab initio* electron and electrostatic properties using GAUSIAN and CRYSTAL, would be also done on the selected compounds. Comparison with the prediction of the preferential interactions using the molecular interaction field (GRID) will be finally performed. This precise characterization of the molecular properties will be used to correlate with the potent biological properties of these species. Besides the interest of the tittle compounds, performing experimental charge density studies will represent a real fundamental challenge.

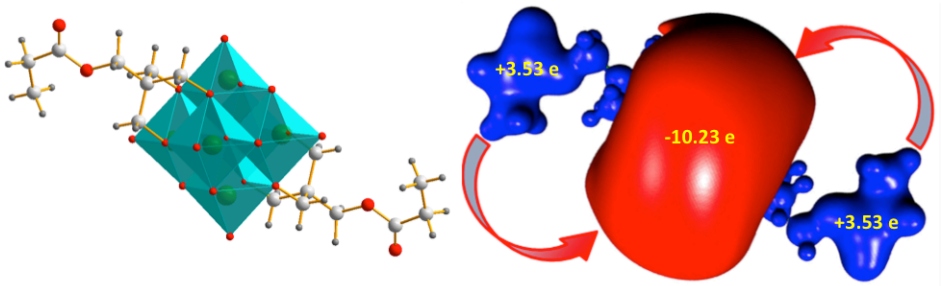

Figure 1. Experimental iso electrostatic potential (e.Å^{-3}) red () blue () of a functionalized polyoxovanadate. The AIM charge is indicated indicating a strong intramolecular charge transger.

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