MS38-O2 Layered and 2D materials: electronic properties and structural instabilities from first principles

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I will present recent work on the understanding of the electronic properties of layered materials and their 2D relatives by means of first principles electronic structure calculations. In particular, I will focus on the correlation between the crystal structure and the electronic properties, with special emphasis on the structural instabilities with an electronic origin. This will be done in connection to recent experimental studies that have been able to demonstrate the presence of charge density waves (CDW) in several 2D materials like $NbSe_2$ and $TiSe_2$. I will also discuss the correlation between the electronic structure and the experimental STM images and STS spectra on some of these systems, which provide crucial insight for the understanding of their CDW and superconducting instabilities.

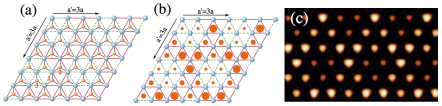

Figure 1. (a) 3x3 CDW structure of single-layer NbSe2. Blue (orange) balls represent Nb (Se) atoms. (b) Schematic STM image predicted for the 3x3 CDW structure taking only into account the height of the different Se atoms. (c) STM image obtained from first principles.

Keywords: 2D materials, DFT, first principles, charge density waves, structural instabilities, electronic structures, low dimensional solids, surfaces.

MS38-O3 Preferred orientation of Li^+ diffusion in nano-$LiMnPO_4$

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Transition metal containing olivine-structured materials, $LiMPO_4$ (M=Fe, Mn, Co, Ni), are considered to be useful as cathode material for lithium ion batteries. They show an excellent structural stability *versus* Li^+ insertion/extraction due to the strong covalent P-O bond[1]. Particularly, $LiMnPO_4$ is attractive because of its high cell voltage (4.1 V vs. Li^+/Li), providing 20 % higher energy density than the commercial $LiFePO_4$. $LiMnPO_4$ consists of slightly distorted LiO_6 and MnO_6 octahedra and PO_4 tetrahedra (Fig. 1)[2]. LiO_6 octahedra are edge-shared with PO_4 tetrahedra. Since the Li^+ diffusion occurs along the *b*-axis via edge-sharing LiO_6 octahedra and hence in one preferred orientation of the crystal structure, a morphology control is important to tune the length of the Li^+ channels in a single particle [3]. We therefore synthesized various shapes and sizes of nano-$LiMnPO_4$ (Fig. 2) to examine the preferred direction of the Li^+ diffusion in single $LiMnPO_4$ particles. The electron diffraction patterns were indexed using transmission electron microscopy to determine the (hkl)-planes and hence the orientation of the *b*-axis in the nanoparticles. Furthermore, the Li^+ diffusion coefficients were determined using electrochemical techniques. According to our measurements for each different shape of nano-$LiMnPO_4$, the Li^+ diffusion occurs always along the shortest facet dimension in a single nanoparticle. The resulting specific capacity was different depending on the shape of $LiMnPO_4$ particles although the total specific surface areas were the same. This study helps to design the desired shapes and sizes of $LiMnPO_4$ for obtaining high energy Li-ion batteries.

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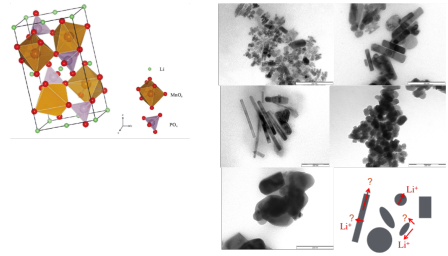

Figure 1. The crystal structure of $LiMnPO_4$ with *P*nma space group. Fig. 2. TEM images show the various shapes and sizes of $LiMnPO_4$ nanoparticles. The scale bar is 200 nm.