

MS41 The use of X-ray, electron and neutron scattering in nanoscience

Chairs: Christian Lehmann, Julian Stangl

MS41-P1 Structure determination and charge density analysis of nanostructured, disordered MoS₂-based layered compounds with organic cations

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Molybdenum disulfide is a layered material demonstrating properties interesting for different applications. A charge transfer onto the MoS₂ layers induces the transformation of semiconductive 2H-modification to "metallic" 1T-MoS₂. The 1T-structure, however, is stable only in the presence of negative charge on the MoS₂ sheets: for example, in intercalation compounds with organic cations. In these compounds, the stabilization of the negative charge on the MoS₂ layers may depend on the interactions between the sulfide layers and organic cations, and the aim of the current study is to determine the structure of such intercalates and the energy of the interactions within them.

Recently [1], we have studied (R,N)MoS₂ (R= H, alkyl) using the "supercell approach" developed by C. Ufer for full-pattern modeling of turbostratically disordered clays. We found that many of intercalation compounds are not fully turbostratic and have short-range correlations between MoS₂ layer positions. These correlations were successfully modeled assuming that the turbostratic disorder is actually exhibited by stable bilayer fragments [2].

In this work, we used this "bilayer-supercell" model to refine the powder patterns of new intercalation compounds of MoS₂ with cations containing aromatic and aliphatic fragments. We obtained the preferred geometry and relative positions of MoS₂ layers and the orientation of aromatic molecules in the interlayer space for compounds with urotropine, phenanthroline and tris-methylphenylammonium cations. We found that compounds with substituted α -amino-naphthalene cations formed turbostratic structure without correlations between MoS₂ layers positions.

The PW-DFT-d calculations based on cell geometries obtained with "bilayer-supercell" approach were used for final verification and charge density determination. Then, we studied the calculated structures within the framework

of R.F.W. Bader's quantum theory of atoms in molecules. Finally, we quantified binding energy of cation-sulfide sheets interactions. To summarize, we found the geometric and energetic characteristics of different weak interactions between organic cations and MoS₂ layers (Fig. 1).

[1] A.S. Goloveshkin, N.D. Lenenko, V.I. Zaikovskii, A.S. Golub, A.A. Korlyukov, I.S. Bushmarinov, *RSC Adv.*, **2015**, *5*, 19206-19212

[2] A.S. Goloveshkin, I.S. Bushmarinov, A.A. Korlyukov, M.I. Buzin, V.I. Zaikovskii, N.D. Lenenko, A.S. Golub, *Langmuir*, **2015**, *31*, 8953-8960

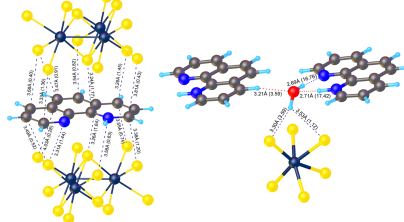


Figure 1. Weak interactions in (PhenH⁺·H₂O)(MoS₂)_{0.10}: π ...S contacts (left part), hydrogen bonds (right part). Distance between non-hydrogen atoms, forming interaction, and its energy in kcal/mole (in brackets) are labeled.

Keywords: molybdenum disulfide, powder diffraction, layered materials, Rietveld refinement, charge density