

MS20-P05 | POWDER XRD STRUCTURE DETERMINATION OF NANOSTRUCTURED, DISORDERED MoS_2 -ETHYLENEDIAMONIUM LAYERED COMPOUND AND MOLECULAR MODELING OF ITS DEPROTONATION REACTIONS

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Unusual, metallic 1T-molybdenum disulfide monolayers showing prospect for application in electrocatalysis can be stabilized by their incorporation into heterolayered systems with organic cations. For these disordered nanomaterials, we recently developed an original approach allowing structure analysis and evaluation of the layers cohesion energy from PXRD data and molecular modeling [1-3]. Here we report an application of this combined approach for new MoS_2 compound, which contains protonated ethylenediamine (EDA) molecules and therefore cation- MoS_2 hydrogen bonding network. By quantifying the binding interaction strength we found that the $\text{NH}\dots\text{S}$ hydrogen bonds have the greatest contribution to the total energy of the specific interactions between organic and inorganic layers (80% of the total energy). By comparison of the energetic characteristics provided by PW-DFT-d calculations for the assembled structure and its “delaminated” and “deprotonated” models, the cohesion energy and behavior of the compound under deprotonation conditions were evaluated. The results show that the compound is stable against deprotonation in the absence of O_2 , while participation of O_2 makes possible partial deprotonation leading to $(\text{EDAH}^+)_{1/6}(\text{MoS}_2)^{1/6-}$ [4].

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