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Structural Rearrangement of Niobium Oxides from Lamellar Phases to Discrete Nanosheets and Nanoscrolls Probed by DFT Calculations JHASHANATH ADHIKARI, LUIS J. SMITH, Clark University — Inorganic niobates $ACa_2Nb_3O_{10}$ (A= H and K) with layered structures are good photocatalytic materials due to their high surface areas accommodating a larger number of active sites and ease of processing through soft chemical techniques like exfoliation and restacking. Alkali metal phases can be ion-exchanged to the acid phase, which in turn can be easily exfoliated to individual nanosheets. The nanosheets can change their form to nanoscrolls with a curled geometry instead of a flat surface. During these morphological transformations, the local structure at the Nb-atom, H-atom and the interface may undergo rearrangement which is responsible for the alteration of properties of the materials. This presentation highlights the preliminary results on these structural modifications (interface variation, stacking of layers, lattice contraction and space group settings) and the possible positions of the proton. Our calculations show that the protons in the acid form are non-bridging and bonded to the same layer oxygen atoms unlike the K-atoms in its parent compound. The Electric field gradient (EFG) is a parameter very sensitive to the electron density around a quadrupolar nucleus ^{2}H and ^{93}Nb that can be detected using NMR. Changes in its magnitude/sign can be correlated to the change in the local environment (bond lengths and angles) around the sites of interest. EFG values from DFT calculations based on the proposed structural models will be used for the characterization of surface O-H bond lengths, H-bonding and Nb-O bond lengths and can be used to interpret NMR studies.

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