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First-Principles Study of Inter-Cage Interactions in Inorganic Molecular Crystals

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Abstract : The inorganic molecular crystal (IMCs) due to their unusual structure has grabbed a lot of attention due to anisotropy in crystal structure. The IMCs consist of the molecular structures joined together via weak forces. Therefore, a difference between the bonding between the inter-cage and intra-cage interactions exists. To look closely at the bonding and interactions, we investigated interactions between two cages of Sb2O3 structure. The interactions were characterized via Extended Transition State-Natural Orbital for Chemical Valence-method (ETS-NOCV), Natural Bond Orbitals (NBO) and Quantum Theory of Atoms in Molecules (QTAIM). The results revealed strong intra-cage covalent bonding while weak van der Waals (vdWs) interactions along inter-cages exits. This structure cannot be termed as layered material although they have anisotropy in bonding and presence of weak vdWs interactions but its bulk is termed as inorganic layered clusters. This is due to the fact that the free standing sheet/films with these materials are not possible. This type of structures may be the most feasible to be used for the system to deal with high pressures and stress bearing materials.

Keywords : inorganic molecular crystals, density functional theory, cages, interactions
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