

## MS21-03 | INTERACTIONS BETWEEN STEREO CHEMICALLY ACTIVE LONE PAIRS IN $\text{MnSb}_2\text{O}_4$

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Stereo chemically active lone pairs are usually treated as text book examples of non-bonding effects and occur in post-transition metal compounds, in which the post-transition metal is in an oxidation state of two lower than its main group number. These oxidation states are found in many technologically important materials, but their structural chemistry is quite intriguing, since the ability to form a lone pair does not always lead to asymmetric coordination. This has been shown to arise from the lone pairs not being chemically inactive, but rather arising from hybridization with the anion valence states.

We here report density functional theory calculations on structurally intriguing  $\text{MnSb}_2\text{O}_4$ , in which the presumed lone pairs on antimony seem to point directly towards each other, suggesting strong interactions between lone pairs. Based on analysis of chemical bonding through orbital based and real space descriptors, we establish the presence of stereo chemically active lone pairs on antimony, and show that they are formed through a similar mechanism to those in binary post-transition metal chalcogenides.

The lone pairs interact through a void space in the structure and are shown to minimize their mutual repulsion by introducing a deflection angle. This deflection angle increases significantly with decreasing Sb-Sb distance introduced by simulating high pressure. This shows the highly destabilizing nature of the lone pair interactions. The chemical bonding in the material is dominated by polar covalent interactions with both significant contributions from charge accumulation in the bonding regions and charge transfer.