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Lattice dynamics of $Bi_2M_2O_7$ (M=Sn, Ti, and Hf) from first principles JIANGANG HE, CRAIG J. FENNIE, School of Applied and Engineering Physics, Cornell University — Insulating bismuth pyrochlores with mixed cations randomly distributed on the B site, $Bi_2MM'O_7$, have been of interest primarily for their dielectric properties. As a way of helping to elucidate the effects of cation disorder from that of the highly polarizable Bi^{3+} lone pair cation, systems like $Bi_2M_2O_7$ (M=Sn, Ti, and Hf) have beed studied. Far from being simple model systems, these single B-site cation materials have been show to display surprisingly complex and local structural distortions. While $Bi_2Sn_2O_7$ and $Bi_2Hf_2O_7$ undergo three and four different phases (where the ground state structure has 352 atoms), $Bi_2Ti_2O_7$ does not show any coherent structural distortions but rather the Bi_2O' simply becomes disordered. In this talk we will present a comparative first-principles study of the lattice instabilities throughout the BZ of the cubic prototype structures of $Bi_2M_2O_7$ (M=Sn, Ti, and Hf) . We then use the eigenvectors of the identified unstable force constants to perform a systematic search over all possible subgroup structure, performing full structural relaxations thereby constructing a picture of the energy landscape. Finally we studied the effect of biaxial strain along [100], [110], and [111].

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