Comparative First Principles Study of $ATiO_3$ Provskite Oxides (A=Ba, Sr, and Pb)

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A comparative study of the structure of $BaTiO_3$, $SrTiO_3$, and $PbTiO_3$ perovskite oxides is performed in order to identify the atomic factors governing the occurrence a ferroelectric or antiferroelectric (rotating-type) phase transition in $ATiO_3$ perovskite oxides. The variational-X α molecular orbital method is employed to calculate the electronic structures of $BaTiO_3$, $SrTiO_3$, and $PbTiO_3$ in a cubic lattice. The changes in the strength of the A-O (A=Ba, Sr, andPB) and Ti-O covalent interactions are determined as a function of the rotation angle of TiO_6 actahedron and the ferroelectric displacement of Ti and O. A comparison of the calculated results indicates that the rotation of TiO_6 octahedron and the ferroelectric displacement are dominated by the A-O and Ti-O covalent interactions, and that the type of phase transition that occurs (ferroelectric and antiferroelectric) in these perovskite oxides is governed by the delicate balance between the strength of the A-O and Ti-O covalent interactions.

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