Electronic structure calculations of $ATiO_3$ perovskite oxides (A=Ba, Sr, and Pb)

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We performed a comparative study of the electronic structures of $BaTiO_3$, $SiTiO_3$, and $PbTiO_3$ to discuss the atomistic factors distinguishing whether a ferroelectric transition takes place or an antoferrodistortive (rotating-type) phase transition does, in $ATiO_3$ perovskite oxides using the Discrete Variational Xα (DV-Xα) molecular orbital method. We have calculated the electronic structures of $BaTiO_3$, $SrTiO_3$, and $PbTiO_3$ in a cubic lattice. We evaluated the changes in the strength of the A-O (between A site atom and O) and Ti-O (between Ti and O) covalent interactions as a function of the rotation angle of TiO_6 octahedron and the ferroelectric displacement of Ti and O. From a comparison of calculated results, we discussed the possibilities of the rotation of TiO_6 octahedron and the ferroelectric displacement which are dominated by the A-O and Ti-O covalent interactions. Our results suggest that whether a ferroelectric phase transitions takes place or an antiferrodistorvite phase transition does is due to the delicate balance between the A-O and Ti-O covalent interactions.