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Title Molecular Orbital Calculation on Lead-Free Perovskite Compounds for Efficient Use of Alkaline and Alkaline-Earth Metals

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Abstract: Effective ionic charges of lead-free perovskite dielectric complex compounds have been investigated with molecular orbital calculation. The base model is of a doubled perovskite cluster; it consists of octahedral oxygen cages with a transition metal ion of titanium, niobium or zirconium located at each of their centers, and alkali and/or alkaline earth metal ions located at a body center, corners, edge centers, face centers of the cluster. The results show significant covalent bonds between the transition metals and the oxygens, and also the alkali metal, especially sodium and the oxygen, while quite weak covalency of alkaline earth metals. The calculation has also been done with replacing some of the oxygens with chlorines or with fluorine enhances covalency of the transition metals. These trends provide good guidelines to design properties of lead-free perovskite piezoelectrics based on ubiquitous sodium use.

Keywords: Perovskite; Dielectrics; Piezoelectrics; Ferroelectrics; Molecular orbital calculation

Graphical Abstract: