

1 Special Issue “Multifunctional Crystal Materials with Non-centrosymmetry: Piezoelectric and Nonlinear
2 Optical Properties and Their Applications”

3 Title Molecular Orbital Calculation on Lead-Free 4 Perovskite Compounds for Efficient Use of Alkaline 5 and Alkaline-Earth Metals

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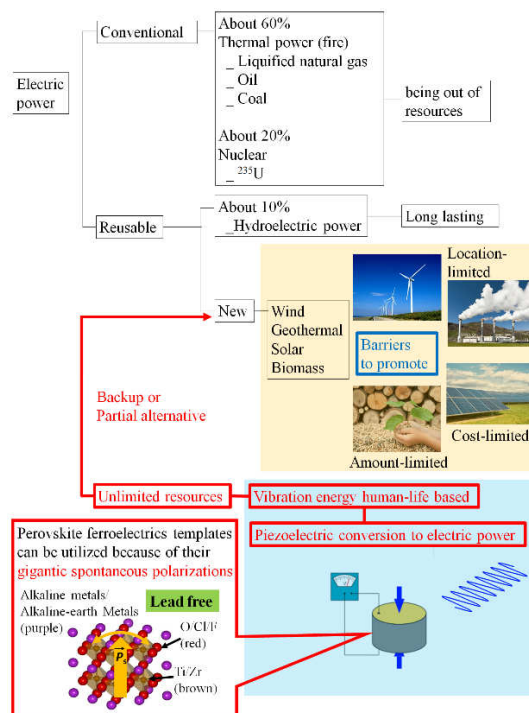
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12 **Abstract:** Effective ionic charges of lead-free perovskite dielectric complex compounds have been
13 investigated with molecular orbital calculation. The base model is of a doubled perovskite cluster;
14 it consists of octahedral oxygen cages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

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

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Graphical Abstract:



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