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Electronic and vibrational properties of tungsten-bronze niobates

MARCO FORNARI, Dept. of Physics, Central Michigan University — We investigated the electronic and vibrational properties of complex niobates with tetragonal tungsten-bronze structure. Our first principles results show that, in $PbNb_2O_6$, the largest contribution to the polarization is from the four 15-coordinates Pb sites (A^{XV}). The interaction between these sites favors the orthorhombic ground-state. The substitution of Ba on the A^{XV} site drives the system to a tetragonal phase forming a morphotropic phase boundary. Replacing Ba with Pb breaks the cooperative behavior a the origin of the orthorhombic phase. Octahedral rotations do not seem to play a significant role even if they influence the energetic of the position of Pb in the A^{XV} cage. Chemical substitutions are tried to explore novel ferroelectric materials.

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