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$_2$O$_6$, 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 at 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.