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Large ferroelectric polarization in the new double perovskite $NaLaMnWO_6$ induced by non-polar instabilities TETSUYA FUKUSHIMA, Graduate School of Engineering Science, Osaka University, 1-3 Machikaneyama, Toyonaka, Osaka 560-8531, Japan, ALESSANDRO STROPPA, SILVIA PICOZZI, Consiglio Nazionale delle Ricerche-Institute for Superconducting and Innovative Materials and Devices (CNR-SPIN), 67100 L'Aquila, Italy, J. MANUEL PEREZ-MATO, Dept de Física de la Materia Condensada, Facultad de Ciencia y Tecnología, Universidad del País Vasco, Apartado 644, E-48080 Bilbao, Spain — Based on density functional theory and group theoretical analysis, we have studied $NaLaMnWO_6$ compound. At low temperature, the structure has monoclinic $P2_1$ symmetry, with layered ordering of the Na and La ions and rocksalt ordering of Mn and W ions. By comparing the low symmetry structure with a parent phase of $P4/nmm$ symmetry, two distortion modes are found dominant. They correspond to MnO_6 and WO_6 octahedron tilt modes, often found in many simple perovskites. While in the latter these common tilting instabilities yield non-polar phases, in $NaLaMnWO_6$ the additional presence of the Na-La cation ordering is sufficient to make these rigid unit modes a source of the ferroelectricity. Through a trilinear coupling with the two unstable tilting modes, a polar distortion is induced, although the system has no intrinsic polar instability. The calculated electric polarization is as large as 16 $\mu C/cm^2$. Despite its secondary character, this polarization is coupled with the dominant tilting modes and its switching is bound to produce the switching of one of two tilts, enhancing in this way a possible interaction with the magnetic ordering.

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