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Abstract

In this work, the structural, electronic, elastic and vibrational properties of orthorhombic *Pmnm* $NaNb_3O_8$ are investigated by means of *ab initio* total energy calculations. The obtained structural parameters are in good agreement with experimental data available at zero pressure. Furthermore, we study the pressure dependence of lattice parameters, bond lengths and bulk moduli of the constituent polyhedra. The electronic band structure is discussed from the density of states and the gap evolution under pressure is analyzed. The change of the elastic constants and the major elastic moduli, with the pressure are described, and several anisotropy indices are evaluated. Frequency, symmetry, pressure coefficients and Grüneisen parameters of phonon modes are reported. We discuss also the mechanical and dynamical stability and we conclude that the compound is dynamically unstable above 5.7 GPa.