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# Ab initio study of the strain-mode coupling in SrBi2Nb2O9

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The Aurivillius compound SrBi2Nb2O9 (SBN) has commonly been considered as a potential candidate for nonvolatile memories, and as a consequence, it has been thoroughly investigated both experimentally [1-3] and computationally [4,5]. The phase diagram of SBN is governed by three relevant distortions, and it has been shown that the trilinear coupling among them stabilizes the ferroelectric ground state [4-6]. An analogous critical influence of the trilinear coupling is also observed in the isomorphous SrBi2Ta2O9 (SBT), where slight differences in the mode interplay induce the presence of an intermediate non-polar phase [3,5,6].

In this work we evaluate by ab initio calculations the couplings of the two components of the strain tensor that do not break the parent tetragonal symmetry with the three relevant symmetry adapted modes. We find that the three modes show significant couplings with strain. Elastic enthalpy is also calculated and we find that a particular combination of applied stress and misfit strain can be used to produce an enhancement of the spontaneous polarization as obtained in other materials [7].

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