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On the origin of the polymorphic phase transition in KNN MARCO FORNARI, Central Michigan University, SAMED HALILOV, Massachusetts Institute of Technology, BORIS KOZINSKY, Robert Bosch LLC, NICOLA MARZARI, Massachusetts Institute of Technology — The discovery of outstanding piezoelectric performance in perovkiste niobates alloys has pointed to these materials as viable lead-free substitutes for enviromentally sound transducers and actuators. Similarly to PZT (the solid solution between $PbTiO_3$ and $PbZrO_3$) the large electromechanical coupling in niobates has been originally linked to a morphotropic phase boundary (MPB) that involves a tetragonal phase formed at room temperature when 1-7% of Li is inserted in $K_xNa_{1-x}NbO_3$ (KNN) with $x \simeq 0.5$. More recently an alternative explanation based on polymorphic phase transition (PPT) was proposed that equally justifies the enhanced piezoelectric constants and points to lack of stability of the electromechanical response as a function of temperature. We have performed first principles density functional calculations to characterize the role of the different chemical components and the local structure near Li atoms. We will discuss Li-Na interaction as the key mechanism that lead to PPT and we will point to specific consequences of the local structure in KNN on the temperature dependence.

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