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Local ordering and structural instabilities in (Na,Bi)TiO_3 perovskites SAHAK PETROSYAN, Massachusetts Institute of Technology, MARCO FORNARI, Central Michigan University, BORIS KOZINSKY, Bosch GmbH, NICOLA MARZARI, GERBRAND CEDER, Massachusetts Institute of Technology — Density functional theory is used to predict structural and electronic properties of lead-free piezoelectric titanate (Na,Bi)TiO_3. We studied the energetics of different phases in the phase diagram and investigated the tendency to local ordering on the A-site. In order to elucidate the mechanism for the phase transitions and the piezoelectric performance we also probed the dependence of ferrodistortive and antiferrodistortive instabilities upon pressure and chemical substitutions. Our results point to local tetragonal ordering and provide insight on possible strategies to improve the electromechanical properties.

Sahak Petrosyan
Massachusetts Institute of Technology

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