

Abstract Submitted  
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**Understanding the role of A-site and B-site cations on piezoelectric instability in lead-free (1-x) BaTiO<sub>3</sub> - xA(Cu<sub>1/3</sub>Nb<sub>2/3</sub>)O<sub>3</sub> (A = Sr, Ca, Ba) solid solutions**<sup>1</sup> DEEPAM MAURYA, YUAN ZHOU, SHASHANK PRIYA, Center for Energy Harvesting Materials and Systems (CEHMS), Bio-Inspired Materials and Devices Laboratory (BMDL), Virginia Tech, Blacksburg, VA 24061 — This study provides fundamental understanding of the enhanced piezoelectric instability in lead-free piezoelectric (1-x) BaTiO<sub>3</sub>-xA(Cu<sub>1/3</sub>Nb<sub>2/3</sub>)O<sub>3</sub> (A: Sr, Ba and Ca and x = 0.0-0.03) solid solutions. These compositions were found to exhibit large longitudinal piezoelectric constant ( $d_{33}$ ) of  $\sim 330$  pC/N and electromechanical planar coupling constant ( $kp$ )  $\sim 46\%$  at room temperature. The X-ray diffraction coupled with atomic pair distribution functions (*PDF*)s indicated increase in local polarization. Raman scattering and electron paramagnetic resonance (EPR) analysis revealed that substitutions on A and B-site both substantially perturbed the local octahedral dynamics and resulted in localized nano polar regions with lower symmetry. The presence of nano domains and local structural distortions smears the Curie peak resulting in diffuse order-disorder type phase transitions. The effect of these distortions on the variations in physical property was modeled and analyzed within the context of nanodomains and phase transitions. \*spriya@vt.edu

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