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**First-principles studies of low tolerance factor perovskites** SUNG GU KANG, CRAIG J. FENNIE, School of Applied and Engineering Physics, Cornell University — Most perovskites form in the non-polar  $Pnma$  structure, however, materials found in the polar subgroup of this structure, e.g., space group  $Pna2_1$ , are rare. Here we study from first principles the structural and vibrational properties of twelve materials that span a wide range of tolerance factors ( $MgSnO_3$ ,  $ZnSnO_3$ ,  $MgTiO_3$ ,  $ZnTiO_3$ ,  $MgGeO_3$ ,  $ZnGeO_3$ ,  $CdSnO_3$ ,  $CaSnO_3$ ,  $CdTiO_3$ ,  $CaTiO_3$ ,  $CdGeO_3$ , and  $CaGeO_3$ ). We illustrate how low tolerance factor materials that have been artificially constrained to the  $Pnma$  structure do in fact display ferroelectric instabilities. Insight is gained by further studying the energetics for each material in the ilmenite, lithium niobate, and perovskite structures over a wide pressure range. Our first-principles results are shown to correlate with physical descriptors, such as tolerance factor, ionic radii, and electronegativity. The rationalized rules from our data analysis will guide to design the new ferroelectric/functional materials.

Sung Gu Kang  
School of Applied and Engineering Physics, Cornell University

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