Ideal Nanocheckerboard $\text{BiFeO}_3 - \text{BiMnO}_3$ from First Principles

LUCIA PALOVA, KARIN RABE, PREMALA CHANDRA, Rutgers University — Motivated by recent nanocheckerboard patternings of oxide materials, we use first principles calculations to characterize a prototypical atomic-scale checkerboard of $\text{BiFeO}_3 - \text{BiMnO}_3$ and to compare its properties to those of its bulk constituents. We find this checkerboard has a multiferroic ground state with nonzero ferroelectric polarization and a nonzero magnetic moment, thereby combining desirable features of bulk $\text{BiFeO}_3$ and $\text{BiMnO}_3$. Unlike either of its parent compounds, structural distortion of the checkerboard stabilizes different magnetic states; this magnetostructural effect can be used to switch between states with zero and nonzero magnetization. The role of oxygen-octahedron rotations and strain in the magnetic ordering of the nanocheckerboard will be examined in detail.