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Ideal Nanocheckerboard $BiFeO_3 - BiMnO_3$ 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 $BiFeO_3 - BiMnO_3$ 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 $BiFeO_3$ and $BiMnO_3$. 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.

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