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Predicting Nanocheckerboards in $ZnMnGaO_4$ Spinel from First Principles MORDECHAI KORNBLUTH, CHRIS A. MARIANETTI, Columbia University — Self-organizing nanocheckerboards raise fascinating questions and present exciting possibilities for ultrahigh-density memory devices. A family of checkerboards fabricated from Mn-based spinels consist of phase-separated Mn-rich (tetragonal) and Mn-poor (cubic) phases. We analyze the earliest example of this family, $ZnMnGaO_4$. Density functional theory (DFT) confirms that the phase separation originates in the Jahn-Teller effect present when Mn ions occupy octahedrally-coordinated sites. DFT calculations demonstrate a strongly preferred (011) interface, which generates checkerboards by geometric considerations. We further investigate both kinetic and thermodynamic limitations in nanocheckerboard composition and size.

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