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**First-Principles Physics of Nanocheckerboard Formation in ZnMnGaO Spinels** MORDECHAI KORNBLUTH, CHRIS MARIANETTI, Columbia University — Using first-principles calculations, we present the physics behind spinel nanocheckerboards in $ZnMn_xGa_{2-x}O_4$. Previously, experiments discovered a group of Mn-based spinels that spontaneously phase-separate into nanocheckerboards. We analyze their origin in the Jahn-Teller (JT) effect, which couples local atomic distortions to an electronic degeneracy (here, the $e_g$ manifold of the Mn d-orbital). Using density functional theory, we show that the interaction between cubic Mn-poor and tetragonal Mn-rich regions causes phase separation, but diffusion prevents the thermodynamic ground state of bulk separation. We demonstrate that the energetics and geometry mandate a nanocheckerboard configuration.

Mordechai Kornbluth
Columbia University

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