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Cooperative phonon effects in the metal-insulator transitions of manganite and nickelate perovskites RICHARD T. BRIERLEY, Yale University, GIAN G. GUZMN VERRI, Universidad de Costa Rica and Argonne National Laboratory, PETER B. LITTLEWOOD, Argonne National Laboratory and The University of Chicago — Metal-insulator transitions in manganite and nickelate perovskites depend on the competition between the electron kinetic energy, which favors the metallic phase, and the electron-phonon coupling and Coulomb interaction, which favor localization. The size of the A-site cation controls the relative rotation of the octahedral structural units of the perovskite in the range of 0 - 15°. This is accompanied by changes in the metal-insulator transition temperature from 0 - 600K. This effect is commonly attributed to modification in the electron bandwidth from changes in orbital overlap.

Although previous theoretical studies of these materials include the electron-phonon interaction, they typically do not consider cooperative phonon effects. Using a phenomenological model of the perovskite structure, we show that the long-range anisotropic forces arising from inter-site phonon interactions are modulated by changes in the octahedral rotation. We demonstrate using statistical mechanical calculations that these changes in the strain interaction can capture the variation in transition temperature with tolerance factor observed in both the manganites and nickelates.

Richard Brierley
Yale University

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