Abstract Submitted
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Phase Separation and Percolative Insulator-Metal Transition in $LaMnO_3$ Under Pressure: A Gutzwiller Variational Study[1] MOHAMMAD SHERAFATI, Dept. of Physics and Astronomy, University of Missouri, Columbia, SASHI SATPATHY, Department of Physics and Astronomy, University of Missouri, Columbia — We study the pressure-induced insulator-metal transition and phase separation in $LaMnO_3$ (LMO) using the Gutzwiller variational method. Being an insulator at ambient pressure, a long-debated question is whether LMO is a correlation-driven Mott insulator or a band insulator driven by the Jahn-Teller (JT) mechanism. Recent Raman measurements of LMO (Ref. 1) reveal a coexistence of domains of JT-distorted and undistorted octahedra between 3 and 34 GPa and indicate a critical threshold for the volume fraction of the latter domains as a herald of the metallic state. To explain these findings, we solve an extended Hubbard model including the JT distortions and cohesive energy as a function of volume for spinless e_g electrons of Mn^{3+} in paramagnetic LMO at room temperature. Our results clearly show a phase separation on both sides of the transition pressure ($P_c = 32$ GPa) where domains of distorted (insulating) and undistorted (metallic) octahedra coexist supporting the percolative nature of the transition. Based on our work, the ground state under pressure is determined by the interplay of both Coulomb and JT interactions and it is predicted that the mixed-phase region extends well above P_c into the metallic region. Ref. : 1) M. Baldini et al., PRL 106, 066402 (2011)

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