

Abstract Submitted
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Theoretical study of charge, spin, and orbital order in half-doped $La_{0.5}Ca_{0.5}MnO_3$.¹ DMITRI VOLJA, WEIGUO YIN, WEI KU, BNL — Deep microscopic insights into the half-doped $La_{0.5}Ca_{0.5}MnO_3$ are obtained with a novel construction of many-body picture derived from LDA+U and Wannier state analysis. Experimentally observed zig-zag orbital order and CE-type magnetic structure is found to have only very weak charge disproportionation. The apparent contradiction between well-defined bridge (3+) and corner (4+) Mn sites and the weak charge disproportionation is resolved naturally with occupied Wannier states centered at 3+ sites extending to 4+ and O-sites (reflecting non-negligible charge-transfer nature of the system.) Contrary to current lore, electron-electron interaction is found crucial to the long-range order in ordering the orbital and the spin. Specific experimental means of verification (e.g.: measurement of pseudospin direction) are suggested.

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