

Abstract Submitted  
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**Weak charge disproportion and leading mechanisms in half-doped manganites.**<sup>1</sup> DMITRI VOLJA, WEI KU, WEI-GUO YIN, Brookhaven National Laboratory — The puzzling very weak charge disproportionation found in half-doped manganites such as  $\text{La}_{1/2}\text{Ca}_{1/2}\text{MnO}_3$  is reconciled with the well-accepted  $\text{Mn}^{3+}/\text{Mn}^{4+}$  picture of charge and orbital orders via our novel first-principles Wannier function analysis. The strong electron itinerancy is found to delocalize the “ $\text{Mn}^{3+}$ ” Wannier states significantly, producing remarkable charge leaking into the “ $\text{Mn}^{4+}$ ” sites. Thus, it is necessary to distinguish for this charge-transfer system actual charge from the occupation number. Finally, a realistic low-energy effective Hamiltonian is derived, revealing the interesting role of electron-electron interactions in the charge and orbital channels, which can be applied to other doping regions including the CMR phase.

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