Weak charge disproportion and leading mechanisms in half-doped manganites.\textsuperscript{1} DMITRI VOLJA, WEI KU, WEI-GUO YIN, Brookhaven National Laboratory — The puzzling very weak charge disproportionation found in half-doped manganites such as La\textsubscript{1/2}Ca\textsubscript{1/2}MnO\textsubscript{3} is reconciled with the well-accepted Mn\textsuperscript{3+}/Mn\textsuperscript{4+} picture of charge and orbital orders via our novel first-principles Wannier function analysis. The strong electron itinerancy is found to delocalize the \textquotedblleft Mn\textsuperscript{3+}\textquotedblright Wannier states significantly, producing remarkable charge leaking into the \textquotedblleft Mn\textsuperscript{4+}\textquotedblright 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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