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Charge Ordering in Half-Doped Manganites: Small Charge Disproportion and Leading Mechanisms

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The apparent contradiction between the recently observed weak charge disproportion and the traditional $\text{Mn}^{3+}/\text{Mn}^{4+}$ picture of the charge-orbital orders in half-doped manganites is resolved by a novel Wannier states analysis of the LDA+ U electronic structure. Strong electron itinerancy in this charge-transfer system significantly delocalizes the occupied low-energy “ Mn^{3+} ” Wannier states such that charge leaks into the Mn^{4+} -sites. Moreover, this feature is found to be generic in doped manganites. Based on a realistic effective Hamiltonian derived from first-principles calculations, we further quantify the leading mechanisms of the charge-orbital orders and find that both electron-lattice and electron-electron interactions are essential. *Preprint arXiv:0704.1834.*

- Prefer Oral Session
 Prefer Poster Session

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