Abstract Submitted
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What is the valence of Mn in GaMnN?[1] RYKY NELSON, Louisiana State University, TOM BERLIJN, Oak Ridge National Laboratory, JUANA MORENO, MARK JARRELL, Louisiana State University, WEI KU, Brookhaven National Laboratory — Motivated by the potential high Curie temperature of GaMnN [1], we investigate the controversial Mn-valence in this diluted magnetic semiconductor. From a first-principles Wannier functions analysis [2] of the high energy Hilbert space we find unambiguously the charge state of Mn to be close to 2+ (d^5), but in a mixed spin configuration with average magnetic moments of 4 μ_B. Using more extended Wannier orbitals to capture the lower-energy physics, we further demonstrate the feasibility of both the effective d^4 description (appropriate to deal with the local magnetic moment and Jahn-Teller distortion), and the effective d^5 description (relevant to study long-range magnetic order). Our derivation highlights the general richness of low-energy sectors in interacting many-body systems and the generic need for multiple effective descriptions, and advocates for a diminished relevance of atomic valence measured by various experimental probes.

[1] Dietl, T., H. Ohno, and F. Matsukura, Phys. Rev. B 63, 195205 (2001).
[2] W. Ku et al., Phys. Rev. Lett. 89, 167204 (2002).

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Ryky Nelson
Louisiana State University

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