Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

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 \(\mu_B\). Using more extended Wannier orbitals to capture the lower-energy physics, we further demonstrate the feasibility of both the effective \(d^3\) 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.


\(^1\)This research is supported in part by LA-SiGMA, NSF Award Number #EPS-1003897. TB was supported by DOE CMCSN and as a Wigner Fellow at the Oak Ridge National Laboratory.

Ryky Nelson
Louisiana State University

Date submitted: 14 Nov 2013

Electronic form version 1.4