

Abstract Submitted
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Optical properties of $\text{Ga}_{1-x}\text{Mn}_x\text{As}$ from large scale ab initio calculations J. JACKSON, R. CARDENAS, G. BESTER, Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany. — The properties of Mn impurities in GaAs are revisited employing a new methodology based on atomic effective potentials (AEPs [1]) which yields LDA accuracy at considerably reduced computational expense. We consider the case of very low Mn concentrations that cannot be considered using conventional ab initio methods and discuss the metal/insulator transition in terms of the Mn-d band localization and its interpretation as a shallow acceptor. We discuss practical methods to improve upon the LDA bandgap in GaAs together with the excessive delocalization of the Mn states. Using a configuration-interaction technique we calculate the optical spectra of $\text{Ga}_{1-x}\text{Mn}_x\text{As}$ including the fine-structure (FSS) splitting which is of importance to the development of quantum computing devices based upon magnetic impurities in semiconductors [2].

[1] J. R. Cárdenas and G. Bester, Phys. Rev. B **86**, 115332 (2012)

[2] D. E. Reiter, T. Kuhn, V.M. Axt, Phys. Rev. B **83**, 155322 (2011)

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