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Linear-scaling DFT+U applied to hole localization and Friedel oscillations in very dilute (Ga,Mn)As ARASH MOSTOFI, Imperial College London, DAVID O'REGAN, Swiss Federal Institute of Technology Lausanne (EPFL), NICHOLAS HINE, Imperial College London, MICHAEL PAYNE, University of Cambridge — System-size and strong electronic correlation are two factors inhibiting the routine first-principles simulation of transition-metal doped nanostructures. Tackling these issues simultaneously, we have developed a linear-scaling implementation of the DFT+U method within the ONETEP code,[1] demonstrating scaling upto $7,000$ atoms. Our implementation allows for nonorthogonal projectors,[2] which may be self-consistently optimized.[3] We apply our approach to the prototypical dilute magnetic semiconductor (Ga,Mn)As. The ferromagnetic interaction between distant localized magnetic moments in (Ga,Mn)As is mediated by defect-induced holes, whose long-range character is critical. Our large-scale calculations on $1,728$ atom super-cells enable us to study the localization and symmetry of the magnetization and hole in the very dilute (0.1%) limit, and to analyze the long-range Friedel oscillations.

[1]Hine, Haynes, Mostofi, Skylaris & Payne, *Comp. Phys. Commun.,* **180**, 1041 (2009).
[2]O'Regan, Payne & Mostofi, *PRB* **83**, 245124 (2011).
[3]O'Regan, Hine, Payne & Mostofi, *PRB* **82**, 081102(R) (2010).

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