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First-principles Investigation of the Neutral and Charged Embedded Clustering in Mn doped GaN: Revisited XIANGYUAN CUI, Sydney University, BERNARD DELLEY, Paul Scherrer Institut, ARTHUR J. FREEMAN, Northwestern University, CATHERINE STAMPFL, Sydney University — Based on extensive density functional theory calculations, the spatial distribution and magnetic coupling of Mn atoms in Mn:GaN has been re-investigated by doping up to 5 Mn atoms in large supercells, where both the neutral and selected charged valence states are studied. The Mn atoms are found to have a tendency to form substitutional embedded clusters with the long-range wurtzite structure maintained. While for neutral pair-doping, the coupling is ferromagnetic regardless of the distance and orientation of Mn atoms, for the experimentally observed oxidation charged state $Mn^{2+}(d^5)$, antiferromagnetic coupling becomes favorable. Furthermore, for both neutral and negatively charged states, for larger (than pair) cluster configurations, states containing antiferromagnetic coupling are always favored. The size of supercell and the atomic relaxation are found important. The electrical conductivity of Mn:GaN depends sensitively on the valence charged states, where the oxidation states $Mn^{2+}(d^5)$ exhibit highly insulating character as observed in experiments. Our results highlight the intrinsic complex nature in transition metal doped dilute magnetic semiconductors, and can rationalize some hitherto puzzling experimental observations.

Xiangyuan Cui
Sydney University

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