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【511】Nonempirical hybrid functionals unravel the intricate mechanisms of self-compensation in Mg-doped GaN

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Enforcing the generalized Koopmans' condition, we construct hybrid density functionals which give band gaps of solids as accurate as state-of-the-art GW calculations and are also capable to correctly describe polaronic distortions. Based on this nonempirical formulation, we address the energetics of native point defects and impurities in GaN. Our results show an amphoteric nature of Mg impurity. It behaves like an acceptor when substitutional to Ga and like a double donor when interstitial. This feature leads to Fermi level pinning and accounts for the observed drop-off of the hole concentration of GaN samples with increasing Mg doping. Importantly, these findings highlight a general effect associated to amphoteric defects which is not limited to the specific case of GaN.

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