Magnetism in C- or N-doped MgO and ZnO: A Density Functional Study of Impurity Pairs

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It is shown that substitution of C or N for O recently proposed as a way to create ferromagnetism in otherwise nonmagnetic oxide insulators is curtailed by formation of impurity pairs, and the resultant C2 spin =1 dimers as well as the isoelectronic N2⁺ interact antiferromagnetically in p-type MgO. For Cdoped ZnO, however, we demonstrate using the Heyd-Scuseria-Ernzerhof hybrid functional that a resonance of the spinpolarized C2 ppπ * states with the host conduction band results in a longrange ferromagnetic interaction. Magnetism of openshell impurity molecules is proposed as a possible route to d⁰-ferromagnetism in oxide spintronic materials.

Spin density at C₂ dimers in ZnO.