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

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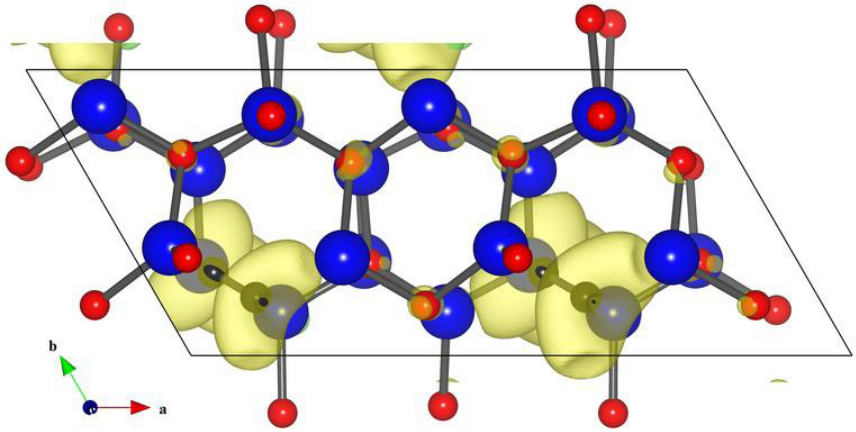
It is shown that substitution of C or N for O recently proposed as a way to create ferromagnetism in otherwise nonmagnetic oxide insulators is curtailed by formation of impurity pairs, and the resultant C2 spin =1 dimers as well as the isoelectronic $N2^{2}$+ interact antiferromagnetically in ptype MgO. 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 d^{0}-ferromagnetism in oxide spintronic materials.



Spin density at C_2 dimers in ZnO.