Abstract Submitted
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Defect pairing and magnetism in C or N-doped MgO and ZnO: a density-functional study[1] PETER KRATZER, University Duisburg-Essen, D-47048 Duisburg, Germany, HUA WU, Universität zu Köln, D-50937 Köln, Germany, SUNG SAKONG, University Duisburg-Essen, XIN-GAO GONG, Fudan University, Shanghai, China, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, D-14195 Berlin, Germany — It is demonstrated that C or N doping recently proposed as a way to create magnetism in otherwise nonmagnetic oxide insulators is curtailed by formation of defect pairs. Our density-functional calculations show that N-N pairing in MgO lowers the energy by 0.4 eV, leading to a nonmagnetic state. C-C pairing is even exothermic by more than 3 eV, and the resultant $(\text{C-C})^{4-}$ molecules with spin=1 couple antiferromagnetically in MgO. However, calculations for C-doped ZnO, when properly treated using the PBE0 hybrid functional, show that the spin-polarized $pp\pi^*$ levels resonate with the host conduction band, which could possibly mediate a long-range ferromagnetic order. Magnetism of open-shell *impurity molecules* is proposed as a possible route to d^0-ferromagnetism in oxide spintronic materials.

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Peter Kratzer
University Duisburg-Essen, D-47048 Germany

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