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Defect-induced Ferromagnetism in Insulators without Magnetic Ions: The Case of Cation Vacancy in CaO[1] JORGE OSORIO-GUILLEN, S. LANY, S.V. BARABASH, ALEX ZUNGER, National Renewable Energy Laboratory — We have investigated by means of first-principle supercell calculations the posibility of ferromagnetism being induced by cation vacancies in non-magnetic oxides in four steps: (*i*) A single neutral Ca vacancy V^0_{Ca} is found to have a magnetic moment of 1.9 μ_B due to its electronic configuration: $(a_1^2\, t_{1+}^3\, e_+^2) t_{1-}^p\, e_-^q$ where, the e_- state is partially occupied ($q \approx 0.5$), leading to a transfer of some hole density to the t_{1-} valence band states ($p \approx 2.5$). (*ii*) The ferromagnetic interaction between two vacancies is found to extend only to four neighbors or less. (*iii*) To achieve magnetic percolation on a fcc lattice with such an interaction range one needs a minimum vacancy concentration of 1.8×10^{21} cm^{-3} (4.9 %). However, (*iv*) due to the high vacancy formation energy even under the most favorable growth conditions one can not obtain at equilibrium more than 10^{18} cm^{-3} vacancies. Thus, a non-equilibrium vacancy-enhancement factor of 10^3 is needed to achieve ferromagnetism in such systems. Comparison with other non-magnetic oxides will be also discussed.

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