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Charge Transfer Ferromagnetism CHRISTOPHER PORTER, The Ohio State University, PLAMEN STAMENOV, Trinity College Dublin, VATSAL DWIVEDI, Indian Institute of Technology, J.M.D. COEY, Trinity College Dublin — A model is developed to describe high-temperature ferromagnetism in defect-ridden materials such as thin films of oxides or nanoparticles. The proposed model consists of a defect-based impurity band and a charge reservoir that can be identified with multivalent dopant cations. Even when the Stoner criterion is not satisfied for the impurity band alone, transfer of charge from the reservoir to the impurity bands may raise the density of states at the Fermi level sufficiently for spin splitting to occur. Whether or not the free energy is lowered by spin splitting depends on the Stoner parameter$I$, the defect bandwidth W, and the energy cost of electron transfer from the reservoir. The free energy minimization has been carried out both in the canonical and grand canonical ensemble. The resulting phase diagrams show half-metallic regions in which spin wave suppression may yield extremely high Cure temperatures of order W. The magnetic phase transitions appear to be first order to within our computational accuracy.

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