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Model for vacancy-induced ferromagnetism in "d0" magnetic oxides TIMOTHY ZIMAN, Institut Laue Langevin and CNRS, Grenoble, GEORGES BOUZERAR, Labo. Louis Neel, CNRS Grenoble — J. Coey has coined the term "d0" ferromagnetism to describe exciting but puzzling effects seen in HfO2, ZrO2 and other oxides. He has also postulated a connection to the occurrence of cation or anion vacancies, which, recent theories indicate, may reasonably lead to the formation of local moments. What has lacked has been a theory which explains why, and at what temperatures, one could expect ferromagnetism. Here we present a simple model for vacancy-based ferromagnetism which permits quantitative estimates of the Curie temperature. The model is based on a random Hubbard model for anions with potentials that represents the occurrence of cation vacancies. By an extension of techniques successfully used to model ferromagnetism in host substituted III-V diluted magnetic semiconductors, we calculate the Curie temperature and dynamical magnetic correlations as a function of the effective strength of the vacancy potential and doping properties, the density of vacancies, as well as the correlation and bandwidth of the host. For physically reasonable parameters this explains large Curie temperatures for rather small concentrations of vacancies.

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