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Frustrating interactions in oxides induced by non-magnetic impurities SHIU LIU, University of California, Irvine, SASHA CHERNYSHEV, University of California, Irvine — An antiferromagnetic host material doped with non-magnetic impurities, such as Zn-doped La_2CuO_4, is generally believed to represent an excellent model case of the site-dilution of a magnetic substance. We demonstrate that there exist a significant qualitative correction to such a picture: an impurity can induce substantial frustrating interactions between spins that are nearest neighbors of the impurity site. Not only this effect explains discrepancies between experimental data and the site-dilution theory, but it could also lead to some important modification of the behavior of doped antiferromagnets close to the percolation. We study the 2D, $S = 1/2$ copper-oxide plane with Zn impurities starting from the microscopic three-band Hubbard model. We show that, for a wide range of the model parameters, the substantial superexchange interactions between the next- and next-next-nearest neighbor Cu spins around the impurity site can be generated via the virtual transitions through the oxygen orbitals. Surprisingly, the interaction across the impurity J''_{Zn} is greater than the next-nearest neighbor interaction J'_{Zn} due to a partial cancellation of the super- and the cyclic exchanges for the latter. This study is completed by the T-matrix calculation of the staggered magnetization $M(x)$ as a function of Zn doping x. The predicted range of J'_{Zn} and J''_{Zn} agrees with the values needed to explain experimental deviation of $M(x)$ from the results of the site-dilution theories.

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