

Abstract Submitted  
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**Impurity induced frustrations in a non-frustrated antiferromagnet** SASHA CHERNYSHEV, SHIU LIU, UC Irvine — Zn substitution for Cu in  $\text{La}_2\text{CuO}_4$  is thought to be an ideal example for a simple site dilution of the antiferromagnetic  $S = 1/2$ , square lattice non-frustrated nearest-neighbor Heisenberg model. We show that starting from the microscopic three-band Hubbard model one obtains quite different, counterintuitive result. Namely, the spinless impurity generates *frustrating* interactions around itself. This is because the oxygen orbitals around Zn impurity site can be still engaged in the virtual transitions which produce substantial superexchange interactions between the Cu spins *across* the impurity site. This effect can explain noticeable discrepancies between the experimental data and theoretical results for the simple site- diluted Heisenberg model.

Alexander Chernyshev  
UC Irvine

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