Impurity induced frustrations in a non-frustrated antiferromagnet
SASHA CHERNYSHEV, SHIU LIU, UC Irvine — Zn substitution for Cu in La$_2$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.