The Jahn-Teller effect in doped LiCuO$_2$ CHRIS MARIANETTI, Columbia University — LiCuO$_2$ displays one of the largest known Jahn-Teller distortions, where Cu$^{3+}$ is in a low spin configuration. Previous density functional theory (DFT) calculations verified the fact that the high spin, non-Jahn-Teller distorted LiCuO$_2$ is a metastable phase. In this work, we use DFT calculations to demonstrate that doping this system with ions that are not Jahn-Teller active allows one to tune the energy difference between the high-spin, non-Jahn-Teller phase and the low-spin, Jahn-Teller phase. This occurs due to the elastic penalty of the non-Jahn-Teller ion in the Jahn-Teller phase. The effect of different non-Jahn-Teller dopants is presented, and the electronic nature of the two respective phases is detailed.