

Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

The Jahn-Teller effect in doped LiCuO₂ CHRIS MARIANETTI,
Columbia University — LiCuO₂ displays one of the largest known Jahn-Teller distortions, where Cu³⁺ is in a low spin configuration. Previous density functional theory (DFT) calculations verified the fact that the high spin, non-Jahn-Teller distorted LiCuO₂ 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.

Chris Marianetti
Columbia University

Date submitted: 21 Nov 2008

Electronic form version 1.4