Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Electron-phonon renormalization in Cuprates. PEIHONG ZHANG, University at Buffalo, SUNY, STEVEN G. LOUIE, MARVIN L. COHEN, UC Berkeley — Electron-phonon (e-ph) renormalization effects in a model cuprate system, CaCuO2, are studied by employing density functional theory based methods. Whereas calculations based on the local spin density approximation (LSDA) predicts negligible e-ph coupling effects of the half-breathing Cu-O bond stretching mode, the inclusion of a screened on-site Coulomb interaction (U) in the LSDA+U calculations greatly enhances the e-ph coupling strength of this mode. The full breathing mode, on the other hand, shows a much weaker e-ph renormalization effect. Enhanced oxygen-p character of the top valence states, together with the (local) antiferromagnetic spin ordering, seems to be responsible for a strong e-ph coupling of the half-breathing mode in the LSDA+U calculations.

Peihong Zhang
University at Buffalo, SUNY

Date submitted: 06 Nov 2006 Electronic form version 1.4