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Electronic structure calculations for the fluctuating-bond model of high-temperature superconductivity. R. A. NISTOR, University of Western Ontario, D. M. NEWS, C. C. TSUEI, G. J. MARTYNA, IBM T. J. Watson Research Center, M. H. MÜSER, University of Western Ontario — High-temperature superconductors (HTS) have been intensely studied for the past 20 years due to their scientific and technological importance. The materials are characterized by square arrays of copper-oxygen-copper bonds. Although several salient features of HTS phenomena have been characterized, a working theory of the underlying physical processes in these materials has been lacking. Collaborators at IBM have recently proposed a model for HTS (Nature Physics **3**, p. 184, 2007), involving a nonlinear coupling of the planar oxygen vibrations to the $d_{x^2-y^2}$ electrons on the coppers. This interaction is modeled as a two-phonon coupling process in the resulting fluctuating-bond model (FBM). In the present work, we investigate the FBM theory by exploring the ability of the oxygens to buckle out of the straight Cu-O-Cu configuration by adjusting the charge on the copper atoms. The study is being conducted using Car-Parrinello simulations to investigate the electronic structure of the materials, and zero temperature single point DFT energy calculations to investigate the floppiness of the oxygen bonds. The aim is to justify, from first principles, the parameterization used in the FBM theory.

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