

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

On the Pairing Instability in Rutile MO_2 L. ANDREA SALGUERO, CRAIG J. FENNIE, School of Applied and Engineering Physics, Cornell University — The metal-dioxide family of compounds such as TiO_2 , SnO_2 , VO_2 , NbO_2 , and WO_2 have been of much recent interest for reasons as diverse as understanding novel correlated electron physics to designing new photo/electro-catalysis. All can be thought of as forming in a prototypical tetragonal “rutile” structure, yet members with unpaired d^1 and d^2 electrons undergo a structural phase transition to a monoclinic, “distorted rutile,” structure. In some cases this metal pairing transition accompanies a metal to insulator transition, the precise role, however, is still not clear. Here we present a comparative first-principles study of the lattice instabilities in d^1 and d^2 MO_2 rutile, paying particular attention to the d^2 system WO_2 , which remains metallic even in the distorted phase. We calculate the phonon dispersion in the tetragonal prototypical structure. Using unstable high symmetry modes as a guide, we calculate the energy surface around the high-symmetry structure and perform full structural relaxations in the distorted ground states. We elucidate the interplay between the electronic structure and the pairing transition and discuss the possibility of controlling it with strain.

L. Andrea Salguero
School of Applied and Engineering Physics, Cornell University

Date submitted: 19 Nov 2010

Electronic form version 1.4