Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Ab-initio electronic structure computation of atomic displacements in an underdoped YBCO superconductor DIDIER DEFONTAINE, Dept. of Materials Science, UC Berkeley, CA 94720-1760, VIDVUDS OZOLINS, Dept. of Materials Science,UCLA, Los Angeles, CA — Recent diffraction studies have shown the existence of lattice modulations in yttrium barium cuprates (YBCO). We show that these modulations are caused by the ordering of O-Cu-O- chains in the CuO planes. Remarkable agreement is illustrated in the case of underdoped YBCO between experimental diffraction patterns of diffuse intensity and satellite intensity obtained from *ab initio* electronic structure calculations. It is suggested that the "stripe" structure of magnetic excitations observed by inelastic neutron scattering originates in the underlying oxygen order described herein.

Didier deFontaine
UC Berkeley

Date submitted: 24 Nov 2004 Electronic form version 1.4