Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

**Structure and Superconductivity of Calcium under Pressure** Z. P. YIN, Dept. of Physics, UC Davis, F. GYGI, Dept. of Applied Science, UC Davis, W. E. PICKETT, Dept. of Physics, UC Davis — The structure, phonon spectrum and electron phonon coupling of Ca under pressure is studied by first principle calculations. Experimentally, Ca at room temperature is simple cubic (SC) at pressure between 30 GPa and 109 GPa and goes to unknown structure above 109GPa. Its superconducting $T_c$ increases significantly in the SC phase, increasing to 23 K at 109 GPa (25 K at 161 GPa). Linear response calculations reveal that SC Ca is horribly unstable in the corresponding pressure range (at T=0). Ab initio molecule dynamics calculations on a 4x4x4 supercell find the SC phase is distorted into a four-atom bcc structure that is dynamically stable in the 40-110 GPa range. At even higher pressure this bcc structure becomes dynamically unstable (imaginary frequencies). T. Ishikawa *et al.* (private communication) proposed an orthorhombic structure around 120 GPa. We confirmed this structure with minor differences of internal parameters. The theoretical x-ray diffraction (XRD) pattern of this structure has very good match with the experimental XRD pattern of the Ca V phase. Our linear response calculations further confirm that it is dynamically stable, and indications of strong electron-phonon coupling in this phase will be presented.

Z. P. Yin
Dept. of Physics, UC Davis

Date submitted: 27 Nov 2007 Electronic form version 1.4