Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Calculations of Superconducting Properties in Yttrium and Calcium under High Pressure[1] DIMITRIOS PAPACONSTANTOPOULOS, LEI SHI, Department of Computational and Data Sciences, George Mason University, Fairfax VA, MICHAEL MEHL, Center for Computational Materials Science, Naval Research Laboratory, Washington DC — We have used first-principles electronic structure calculations to generate the bulk modulus as a function of volume as well as the densities of states and scattering phase shifts at the Fermi level. These quantities were used in conjunction with the rigid-muffin-tin theory of Gaspari and Gyorffy and the McMillan theory to determine the electron-phonon coupling and the superconducting transition temperature for Yttrium and Calcium under high pressures. Our results provide a good interpretation of the measured increase of T_c in these metals.

[1]Supported by the Office of Naval Research.

Dimitrios Papaconstantopoulos
Department of Computational and Data Sciences
George Mason University, Fairfax VA

Date submitted: 21 Nov 2006 Electronic form version 1.4