Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Electrons and phonons in YbC_6 IGOR MAZIN, Naval Reasearch Lab — Electronic structure and selected zone center phonons, as well as the electron-phonon coupling are calculated for a novel intercalated graphite supercoductor, YbC_6, using LDA+U method (fully localized version). The only stable solution either in LDA or in LDA+U is with zero spin and orbital polarization and the 4f band fully occupied. We show that Yb d states are present at the Fermi level and assess a hypothesis that superconductivity may arise from Yb phonons.

Igor Mazin
Naval Reasearch Lab

Date submitted: 29 Nov 2004 Electronic form version 1.4