Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Vibrational spectrum and electron-phonon coupling of doped solid picene from first principles LILIA BOERI, ALASKA SUBEDI, Max Planck Institute for Solid State Physics, Stuttgart — The search for new intercalated hydrocarbon superconductors was initiated by the report of a superconducting critical temperature (T_c) of 18 K in K- and Rb- doped picene ($C_{22}H_{14}$), followed by phenanthrene, coronene and di-benz-picene (27 K). These compounds, formed by justappoxed benzene rings, bear a strong resemblance both to fullerenes and intercalated graphites. Using first-principles linear response calculations have performed calculations of the phonon spectrum and electron-phonon (ep) interaction, we have shown that the coupling of the high-energy C bond-stretching phonons to the π molecular orbitals for a doping of 3 electrons per picene molecule is sufficiently strong to reproduce the experimental Tc of 18 K within Migdal-Eliashberg theory. For hole doping, we predicted a similar coupling leading to a maximum Tc of 6 K. However, we argue that, due to its molecular nature, picene may belong to the same class of strongly correlated *ep* superconductors as fullerides [1]. Our results are in agreement with estimates based on molecular orbital models;we also discuss possible reasons and implications of the discrepancy with linear response calculations that include explicitely the dopant.

Lilia Boeri
Max Planck Institute for Solid State Physics, Stuttgart

Date submitted: 09 Nov 2011 Electronic form version 1.4