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A First-Principles Insight into the Superconductivity of Graphite Intercalation Compounds LILIA BOERI, OLE KROGH ANDERSEN, JUN SUNG KIM, REINHARD KREMER, Max-Planck-Institut fuer Festkoerper-Forschung, Stuttgart, Germany, MATTEO GIANTOMASSI, UPCM, Universite Catholique de Louvain, Louvain-la-Neuve, Belgium, GIOVANNI B. BACHELET, INFM SMC and Dipartimento di Fisica, Universita la Sapienza, Roma, Italy, FERIDON S. RAZAVI, Department of Physics, Brock University, Ontario, Canada — Experimental evidences have estabilished that the recently discovered superconductivity in graphite-intercalation compounds (GICs) CaC_6 and YbC_6 is due to electron-phonon ($e-ph$) coupling. First-principles calculations predict for CaC_6 an intermediate $e-ph$ coupling ($\lambda \sim 0.83$), resulting from intercalant in-plane (I_{xy}) and carbon out-of-plane (C_z) vibrations. Whereas the softening of the I_{xy} modes explains increase of T_c with pressure [1], the presence of the C_z peak is due to an interaction which is "dormant" in pure graphite. A simple analysis of the band structure of the GICs also permits to rule out the possibility of plasmon-meadiated superconductivity[1].

[1] J. S. Kim, L. Boeri, R. K. Kremer, and F. S. Razavi Phys. Rev B, in press and Phys. Rev. Lett. 96, 217002 (2006).

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