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Superconductivity in Alkali-Earth intercalated graphite. MATTEO CALANDRA, FRANCESCO MAURI, IMPMC, Universite de Paris 6 — It has long been known that Graphite intercalated compounds (GICs) can display a superconducting behavior at low temperature. However, until the discovery of YbC_6 and CaC_6, the critical temperatures achieved were typically inferior to 5 Kelvin. Using density functional theory we study superconductivity in AC_6 with A=Mg,Ca,Sr,Ba. We find that at zero pressure Ca, Ba and Sr intercalated graphite are superconducting with critical temperatures (T_c) 11.5, 0.2 K and 3.0 K, respectively. We study the pressure dependence of T_c. We find that the SrC_6 and BaC_6 critical temperatures should be substantially enhanced by pressure. On the contrary, for CaC_6 we find that in the 0 to 5 GPa region, T_c weakly increases with pressure. The increase is much smaller than what shown in several recent experiments. Thus we suggest that in CaC_6 stacking faults or a continous phase transformation,such as an increase in staging could occur at finite pressure. Finally we argue that, although MgC_6 is unstable, the synthesis of intercalated systems of the kind $Mg_xCa_{1-x}C_y$ could lead to higher critical temperatures.

[1] M. Calandra and F. Mauri, Phys. Rev. Lett. **95**, 237002 (2005)
[2] M. Calandra and F. Mauri Phys. Rev. B 74, 094507 (2006)

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