Inducing Superconductivity at the Surface of Hydrogenated Diamond: an ab-initio study

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Superconductivity in boron-doped diamond has been widely studied in the last decade. Although an increment of the boron concentration should lead to an enhancement of the superconducting transition temperature[1] there is a limit to the amount of boron which can be chemically incorporated in the lattice.

A possible solution to this problem (which also avoids the detrimental effect of impurities) is a pure charge doping by means of the electrochemical gating technique. By tuning the applied electric field in a field-effect transistor (FET) geometry - with an ionic liquid instead of the solid dielectric - one can control the surface charge density (and its sign) induced in the material. The use of the ionic liquid allows reaching values of the induced densities between 10^13 and 10^15 cm^-2, depending on the quantum capacitance of the material.

Our aim is to study the possible superconductive phase transition of the hydrogenated diamond [111] surface in the FET geometry by means of ab-initio density functional theory computations within the pseudo-potential plane-wave approximation. In particular, we use a recent model[2] that extends the possibility of the Quantum Espresso software to the calculation of electronic and vibrational properties in the FET configuration. The superconductive critical temperature is then computed using McMillan's semi-empirical model starting from ab-initio electron-phonon matrix elements.

1. E. Bustarret, Phys. Stat. Sol. (a) 205, 997-1008 (2008)
2. T. Sohier, M. Calandra, F. Mauri, Phys. Rev. B 96 (7), 075448 (2017).