Symmetry and electronic structure study of a predicted hybrid graphene-diamond like carbon phase

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Carbon has always attracted attention due to its rich chemistry and the almost complementary properties of the natural phases graphite and diamond. While graphite is a highly anisotropic semi-metal, diamond shows high hardness and thermal conductivity and is a wide-gap insulator. With the discovery of graphene, fullerenes, and carbon nanotubes which resemble properties of the two crystalline phases research on those and novel carbon materials emerged. Since carbon is forming different covalent bonds, there is a multitude of possibilities to create new structures by just combining *sp*, sp^2, and sp^3 bonded carbon. Here we report on the discovery of a new sp^2 and sp^3 bonded carbon structure which can be seen as a crossed graphene structure (see Fig. 1a) providing hybrid properties of graphene and diamond by means of an evolutionary algorithm [1]. We investigated the dynamical stability and elastic and electronic properties (see Fig 1b) of the new carbon phase in detail. For possible identification we provide the theoretical Raman spectrum showing modes which would allow it, to differentiate the structure from other known carbon structures.

[1] S. Bahmann and J. Kortus: *EVO - Evolutionary algrorithm for crystal structure prediction*, Comp. Phys. Comm. **184,** 1618 – 1625 (2013)

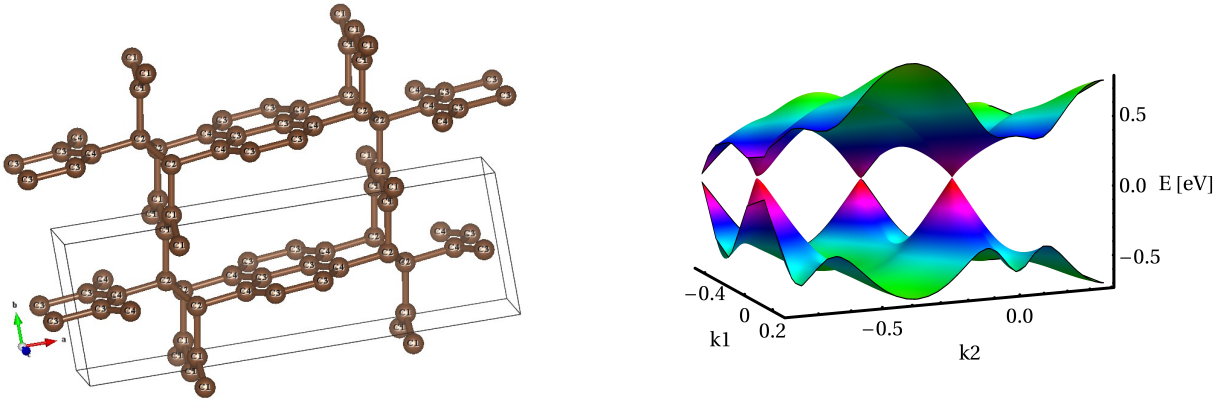

Fig 1: (a) The left side shows the crystal structure of the new sp^2 and sp^3 bonded carbon structure. (b) The right panel displays the electronic band structure close to the Fermi level, where Dirac-like cones similar to graphene are visible.