Understanding the conduction mechanism of carbon foam surfaces

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Carbon foams are periodic structures containing graphene ribbons which are connected with each other along their edges with sp^3 bonds. Cleavage of the bulk structure normal to the connected graphene ribbon edges, leads to either an sp^3- or sp^2-terminated surface, (i.e. terminated by C atoms that were either sp^3 or sp^2 in the bulk, respectively), which are shown in Fig. 1(a) and 1(b).

We performed *ab-initio* calculations using SIESTA and TRAN-SIESTA codes to study the stability, and the electronic and transport properties of foam slabs with either sp^2 or sp^3 terminated surfaces, with and without Hydrogen termination[1]. We find that sp^2 and sp^3 terminated surfaces exhibit metallic and semiconducting behavior, respectively, which occur either with or without Hydrogen termination. Consequently, such behaviors are not related to the surface dangling bonds.

Using Tight Binding calculations in order to understand those different behaviors, we find that the conducting behavior of carbon foam surfaces derives from first- and second-nearest neighbor interactions (f.n.n.i. and s.n.n.i.) between $p_{\parallel}$ orbitals, located at sp^2 sites, which are shown schematically in Fig. 1(c) - 1(e) with solid red and dashed green lines, respectively. Due to the foam topology, f.n.n.i. (see Fig. 1(c)) split the atomic eigenstates E_p to $E_p \pm V_{pp\pi}(1)$, producing a band gap, which turns both sp^3 terminated slabs and the bulk foam to semiconductors. However, $p_{\parallel}$ orbitals located at the sp^2 sites of the sp^2 terminated surfaces, interact only through s.n.n.i. (see Fig. 1(d)), and therefore the atomic eigenstates $E_p = E_F$ do not split, but just broaden around E_p, leading to a metallic system.

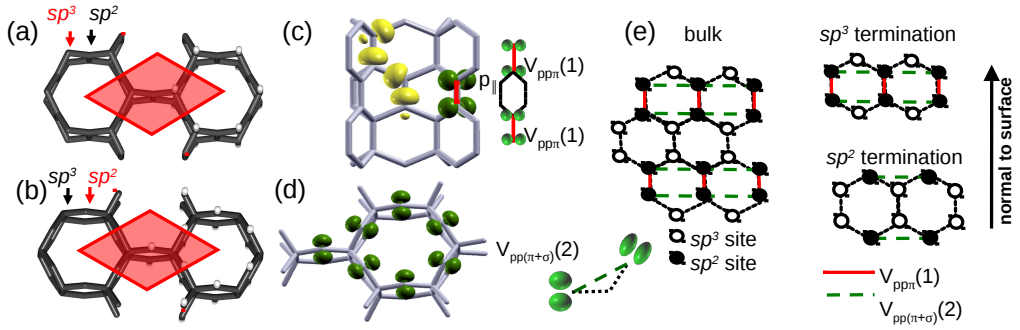

Figure 1: (a) Structure of sp^3 and (b) sp^2 terminated slab. (c) Side and (d) top view with $p_{\parallel}$ orbitals (green). (e) Schematic representation of f.n.n.i. and s.n.n.i

References

[1] Z. Zhu, Z. G.Fthenakis, J. Guan and D. Tománek, Phys. Rev. Lett. **112**, 026803 (2014)

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