Rigorous simulation of carbon-based nano-systems for transistor devices

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Low-dimensional carbon systems, given by atomic clusters (0D), nanotubes (1D), and graphene sheets (2D) are widely investigated for their unique physical properties.
Here, graphene sheets and carbon balls (C60) are considered for rigorous density functional theory (DFT) simulation, in the context, respectively, of graphene-FET and single-electron transistor (SET) devices [1-3] (see Fig. 1). The former has been object of intense study, to assess the potential benefit of the long range ballisticity of charge carriers [4]. The latter are very promising new nanoscale devices, that not only retain their scalability even at the atomic scale, but also base their functioning on quantum phenomena. Extremely high integration and very low power consumption will be the main attributes of such devices. The SET is a type of switching device that uses controlled electron tunneling to amplify current, made from two tunnel junctions that share a common electrode. The only way for electrons in one of the metal electrodes to travel to the other electrode is to tunnel through the insulator. Since tunneling is a discrete process, the electric current passing through the tunnel junction flows in multiples of the charge of a single electron, giving rise to unique current voltage characteristics. The latter are derived by the master equation method [5].

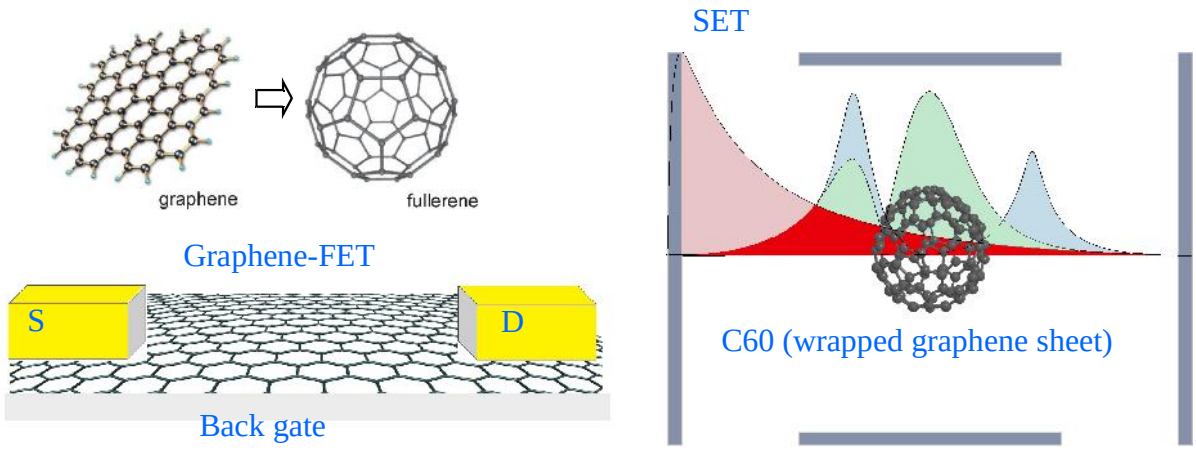

Figure 1. Graphene FET and C60 SET. For the latter, we report a sketch the coupling between an atomic cluster and lateral electrodes, through superposition of electronic wavefunctions and effective potentials.

References

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