Density Functional Theory (DFT): numerical results for molecules and condensed matter

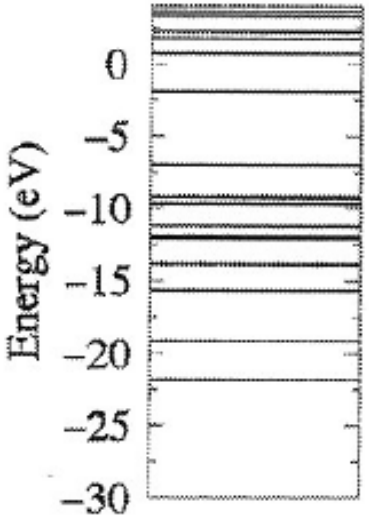
Benzene molecule and carbon nanotube

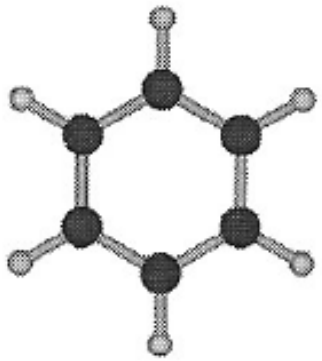
Reference:

Computational Nanoscience

Kalman Varga and Joseph A. Driscoll

Cambridge University Press, 2011





Benzene

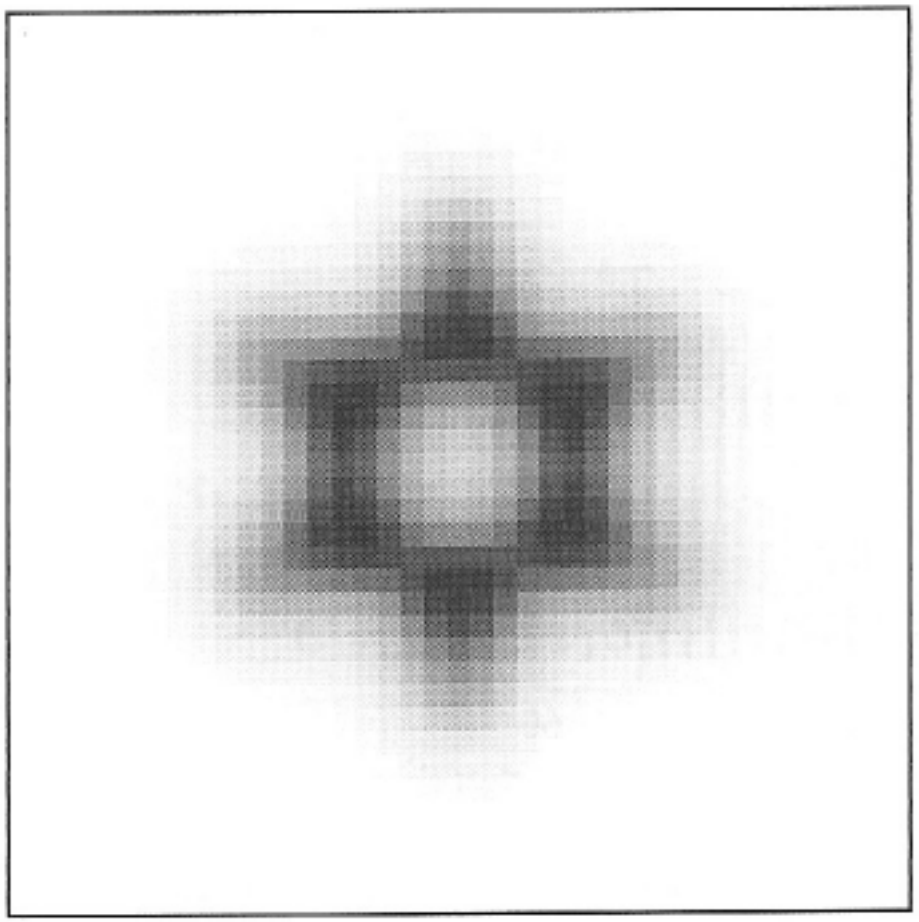


Figure 14.2 Average electron density of a benzene molecule.

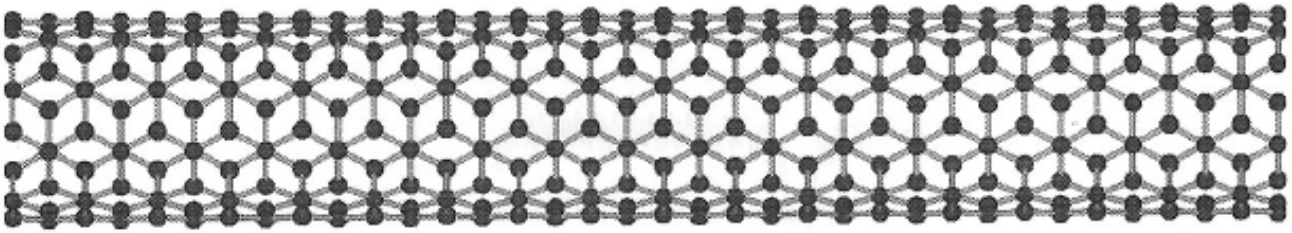


Figure 14.3 Ball and stick model of a (5, 5) carbon nanotube.

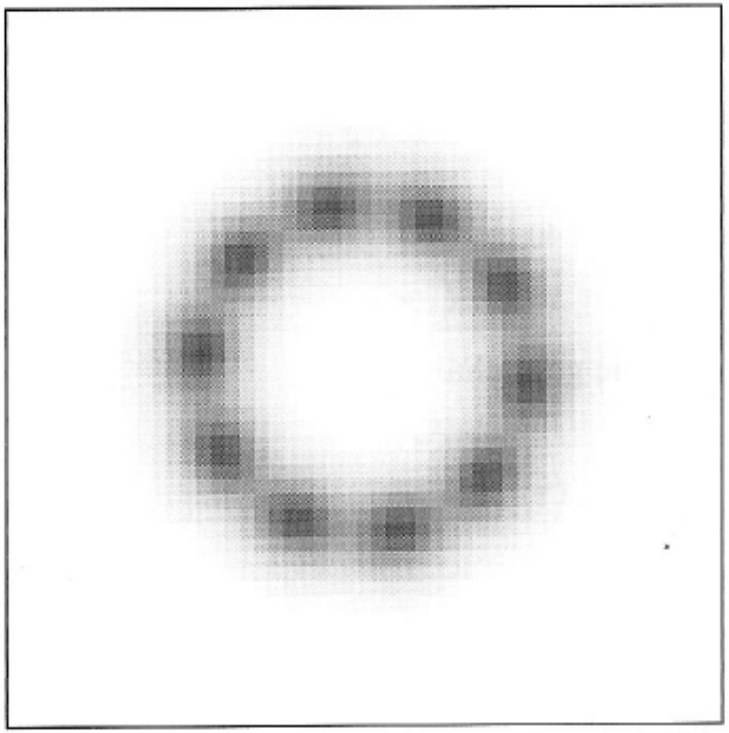


Figure 14.4 Average electron density of a (5, 5) carbon nanotube on a plane perpendicular to the axis of the nanotube.

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Molecular doping of graphene with ammonium groups

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II. METHOD

The results were obtained with the density-functional theory code VASP[12] using ultrasoft pseudopotentials[13] for the valence electrons. We used a local-density approximation (LDA) exchange and correlation (xc) functional[14] and an energy cutoff of 300 eV for the plane-wave basis. For selected configurations we also used a generalized gradient approxi-

The supercells for calculations on a graphene layer contained 160 carbon atoms in a simulation box with in-plane dimensions of 19.65 and 21.27 Å. Total-energy calculations for this case used the Monkhorst-Pack[22] scheme for sampling of the reciprocal space and a $3\times3\times1$ k mesh. Calculations of electronic densities of states (DOS) employed the tetrahedron method[23] and $9 \times 9 \times 2$ grids for k-point sampling. The

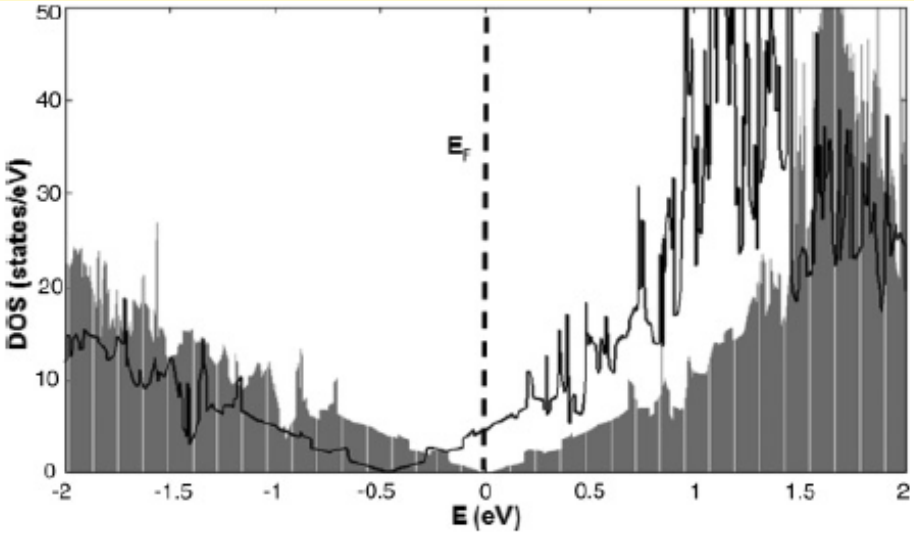

FIG. 1. Electronic density of states (DOS) for graphene with no impurities (shaded area) and with a physisorbed NH_4 group (black solid line). E_F is the Fermi level.

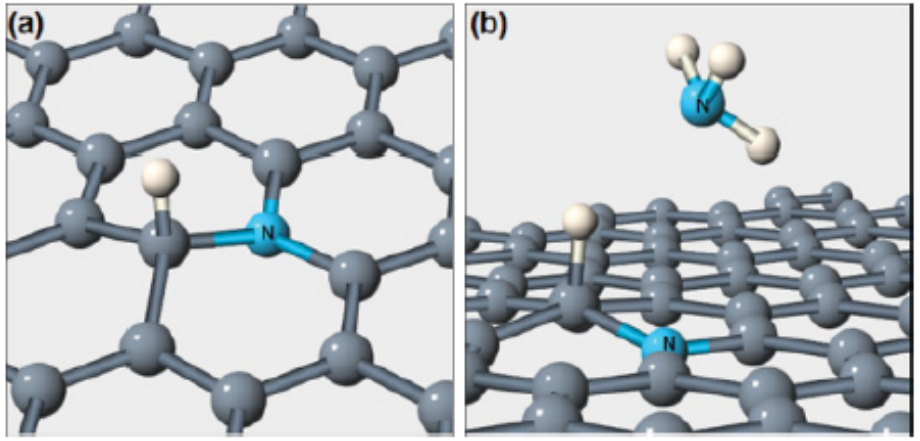

FIG. 2. (Color online) (a) N-H complex: H atom trapped at a substitutional N dopant site of graphene. (b) a NH_3 molecule physisorbed over a N-H complex. [C: gray; N: light gray (cyan); H: white spheres.]