MB-JASS 2007
Nanotechnology and new Materials in Electronics

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MIET Moscow

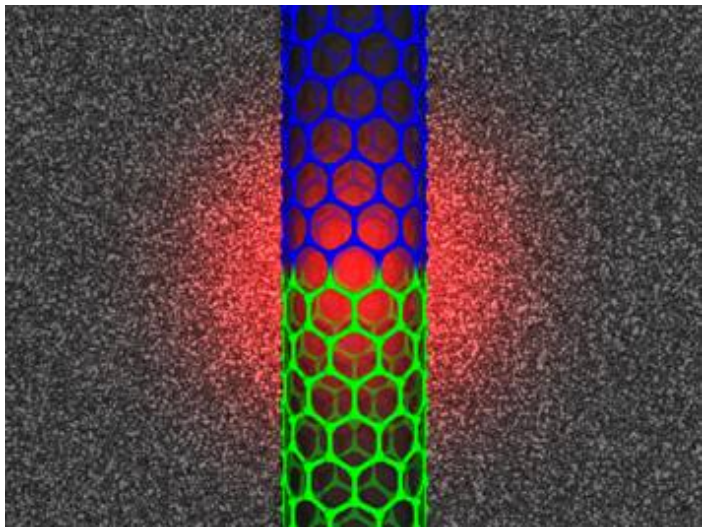

МИЭТ

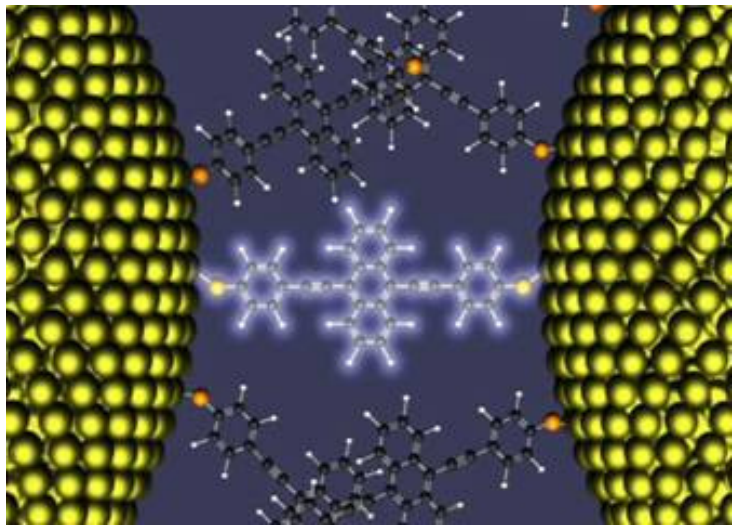
Nanotechnology

New Materials

Quantum Theory of Nanostructures and Materials

Molecular devices





Methods of the self-organization

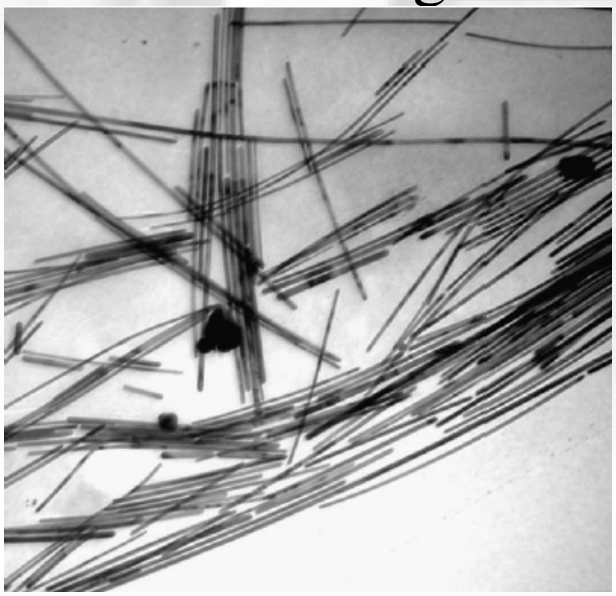
Vapor-liquid-solid growth

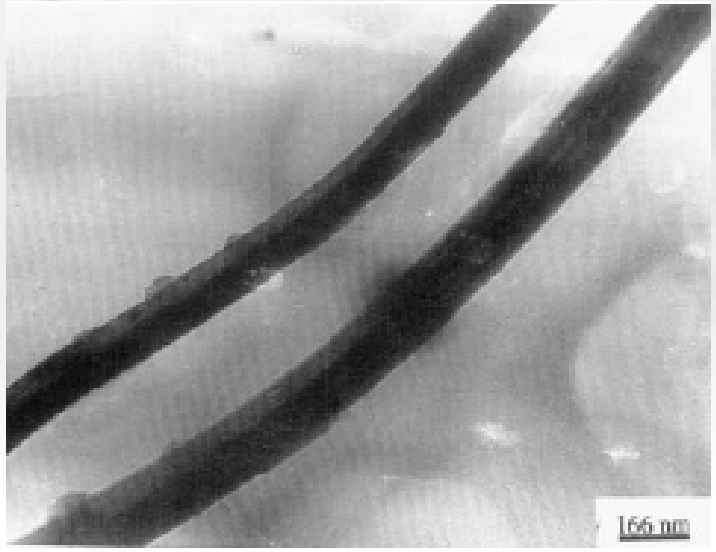
Vapor-solid growth

Solution–liquid–solid growth

Growth with oxide presence

Carbothermal reactions





The TEM images of Ag and CdS nanowires

Tunneling Microscopy

Рис. 11. Внешний вид атомно-силового микроскопа Solver PRO без защитного колпака

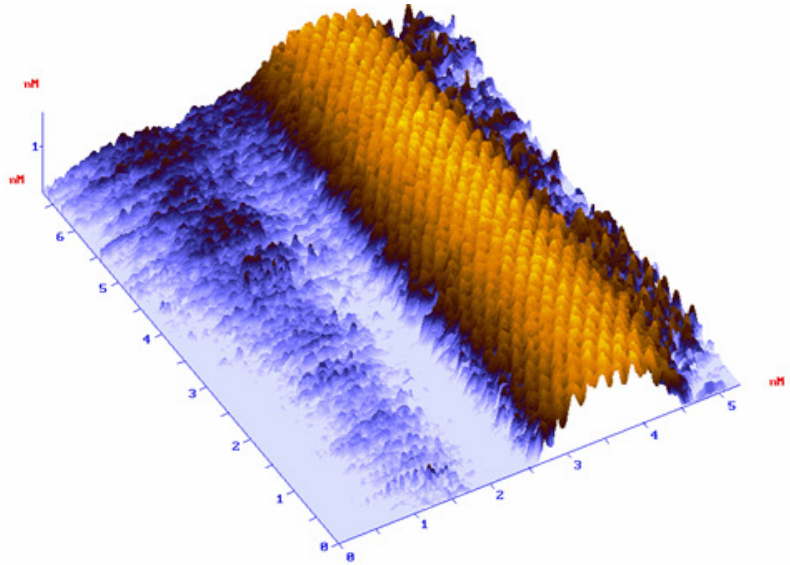


Рис.12. СТМ изображение с атомным разрешением поверхности углеродной нанотрубкина, подложке из пиролитического графита.

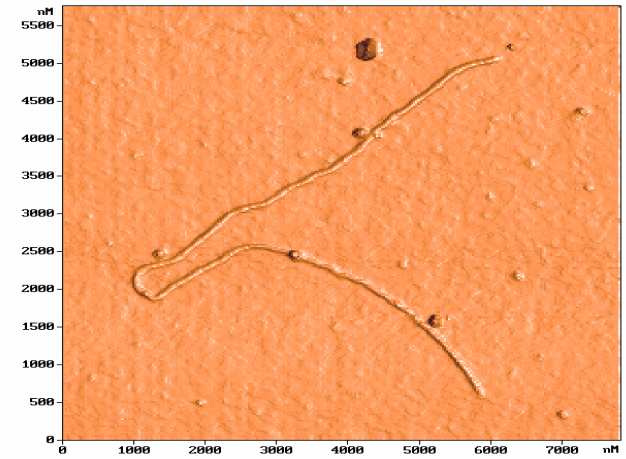
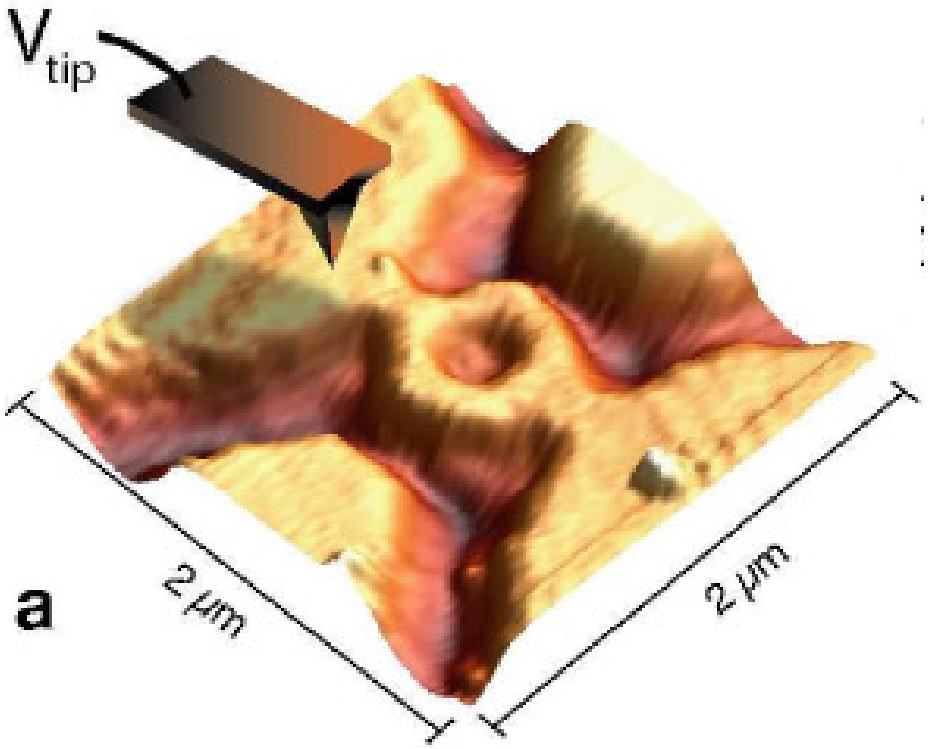
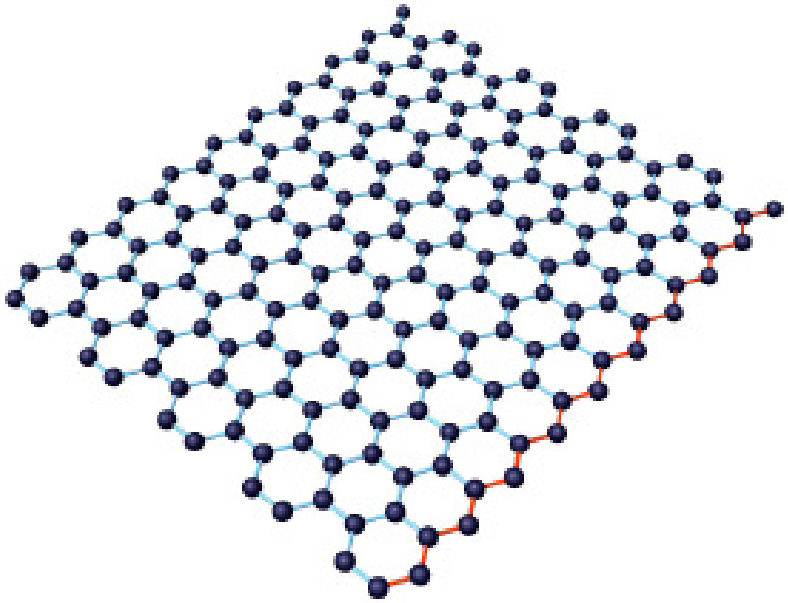


Рис.13. Изображение углеродной нанотрубки в атомно-силовом микроскопе Р-47.

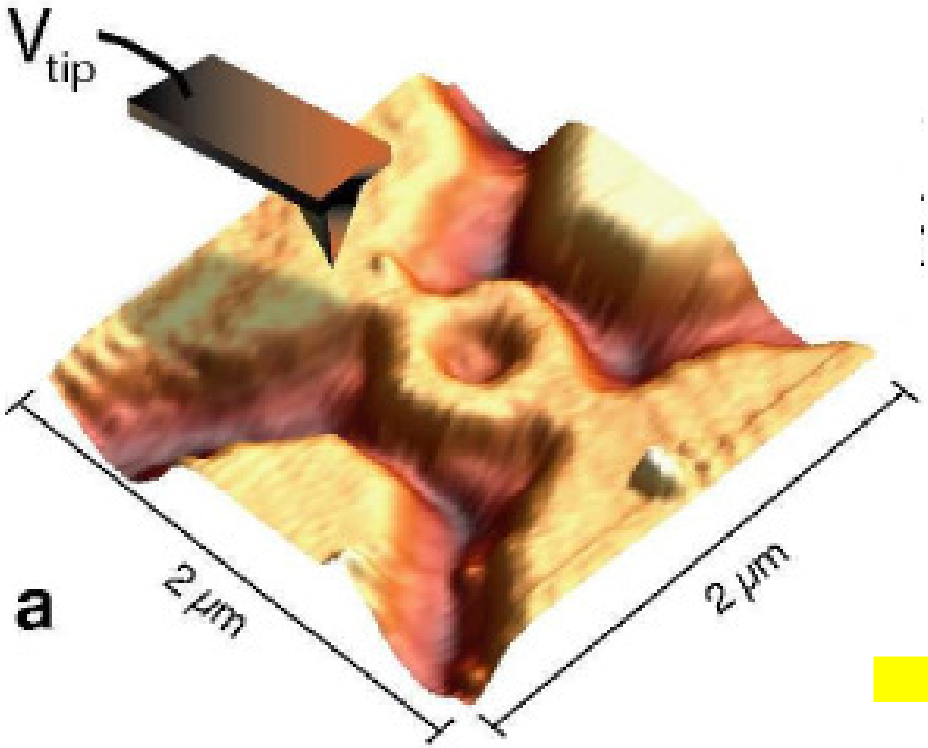
Nanostructure: Quantum ring

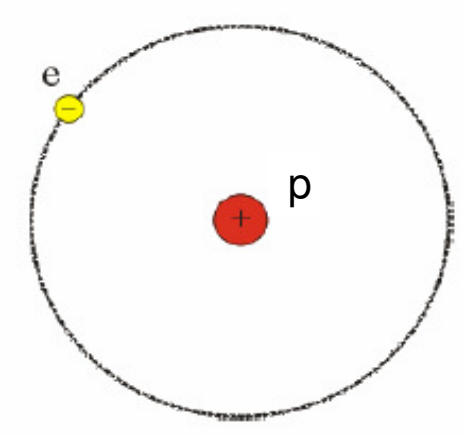


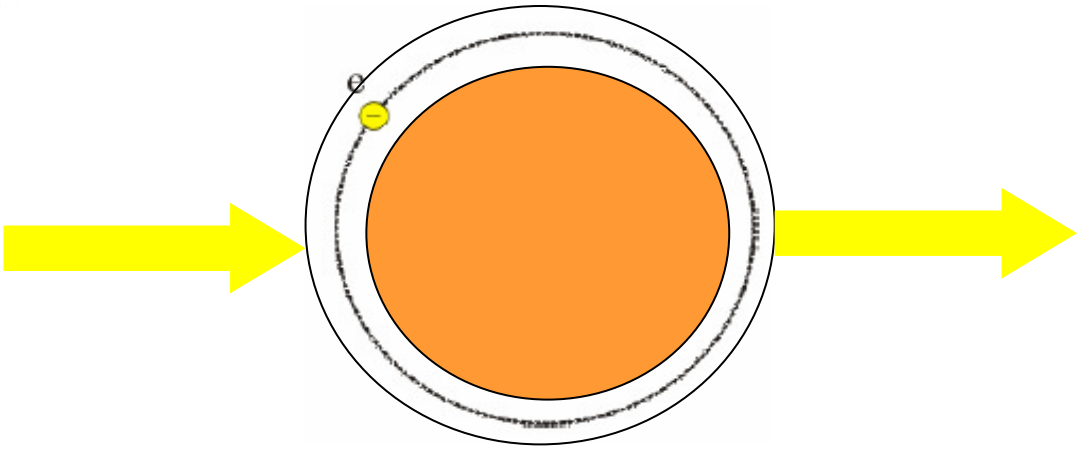
New material: Graphene



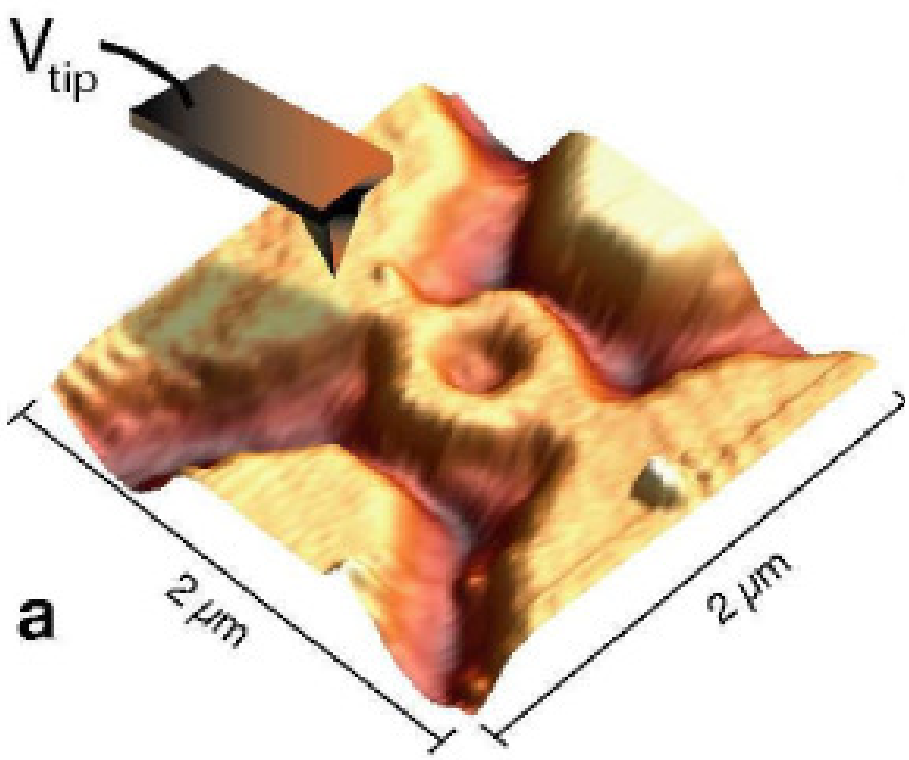
Quantum ring

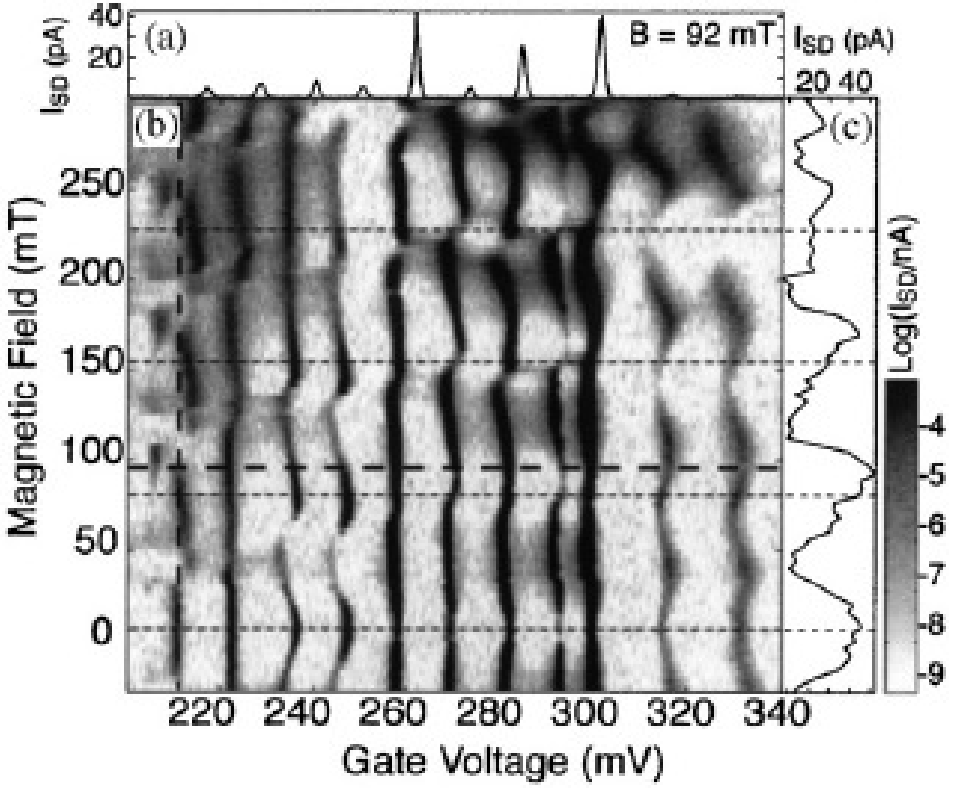




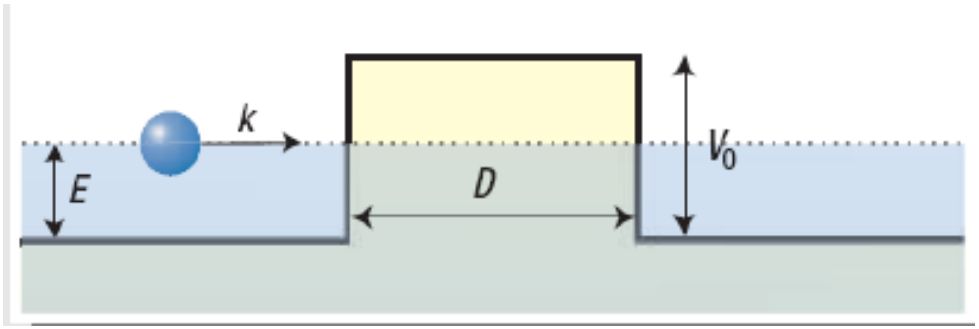


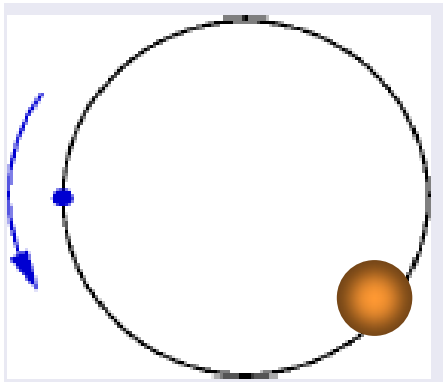
Quantum rings

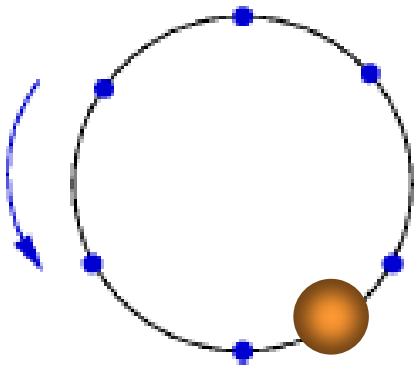




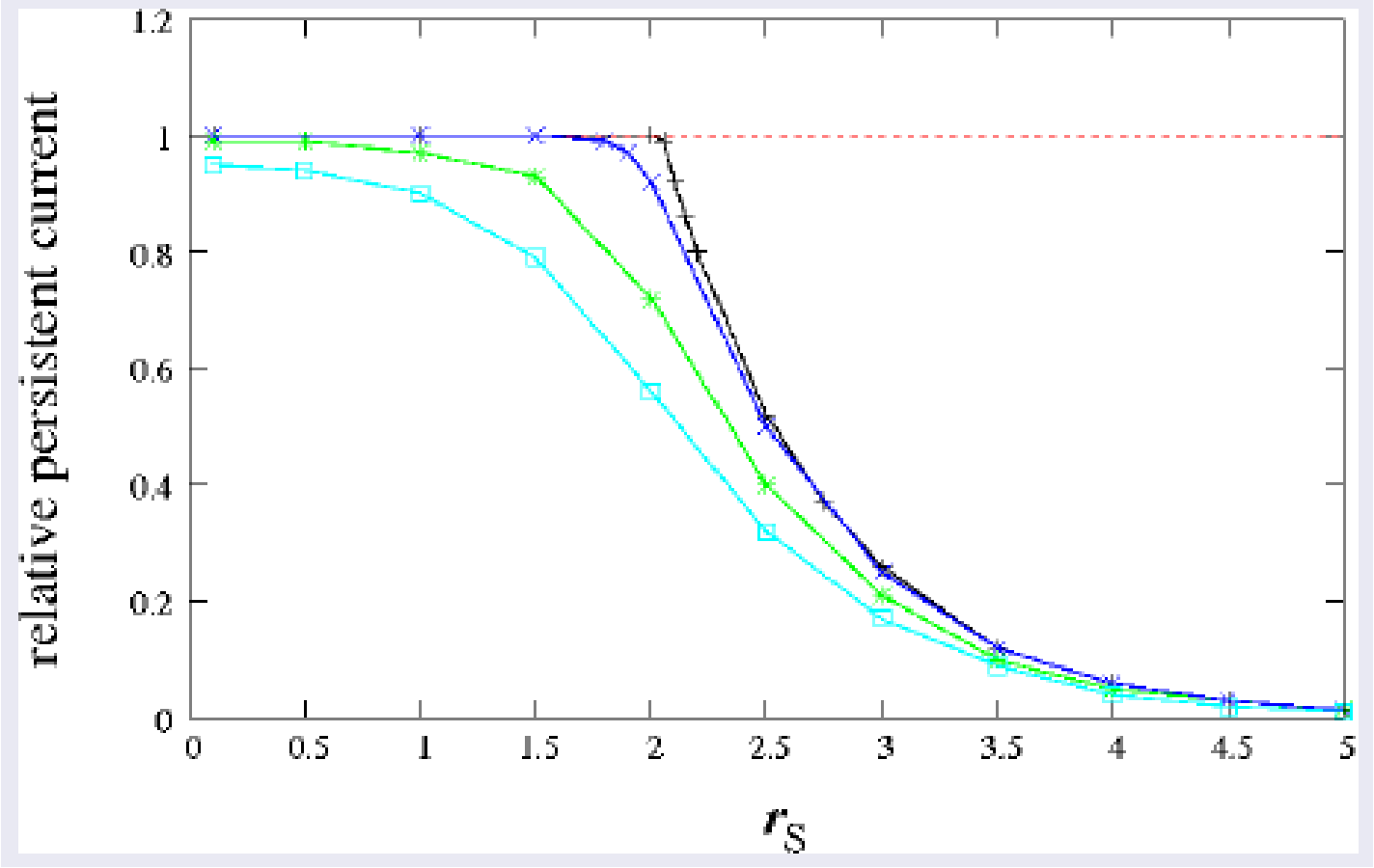
Quantum tunneling







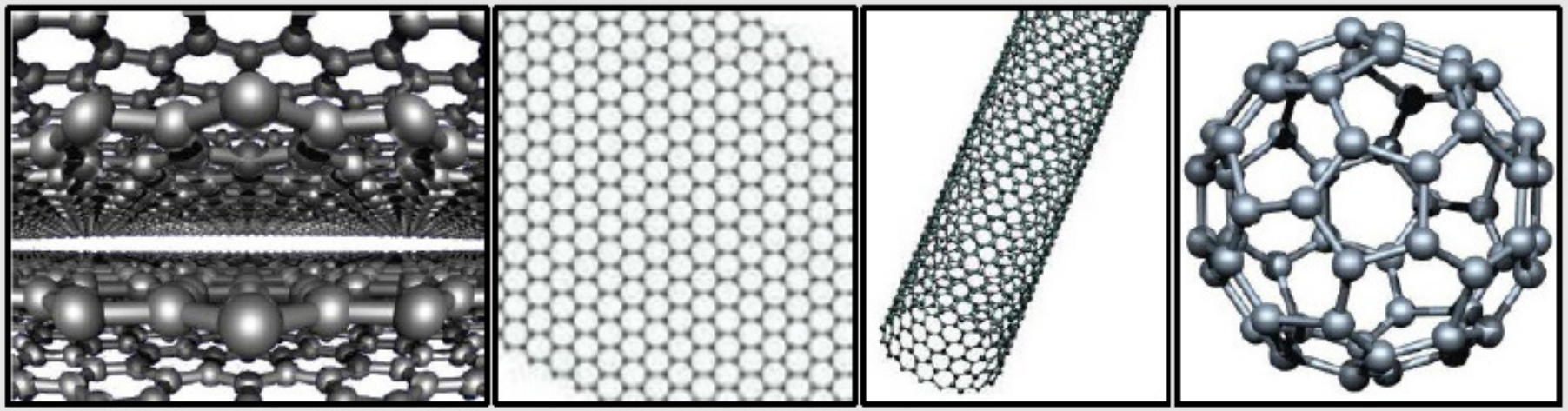
Electron crystallization on a ring: calculated persistent current



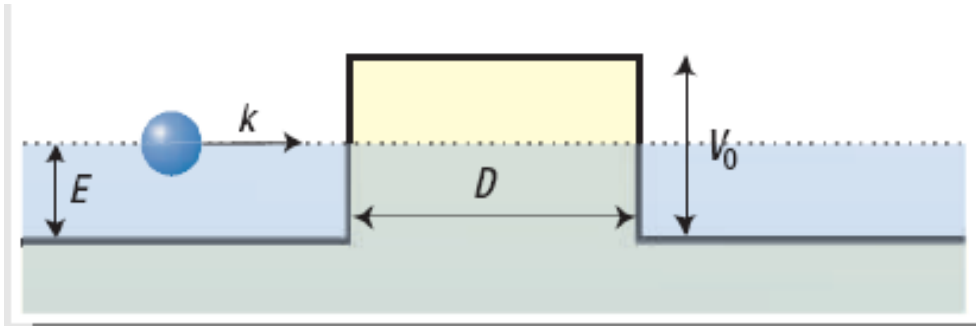
From Graphite to Graphene

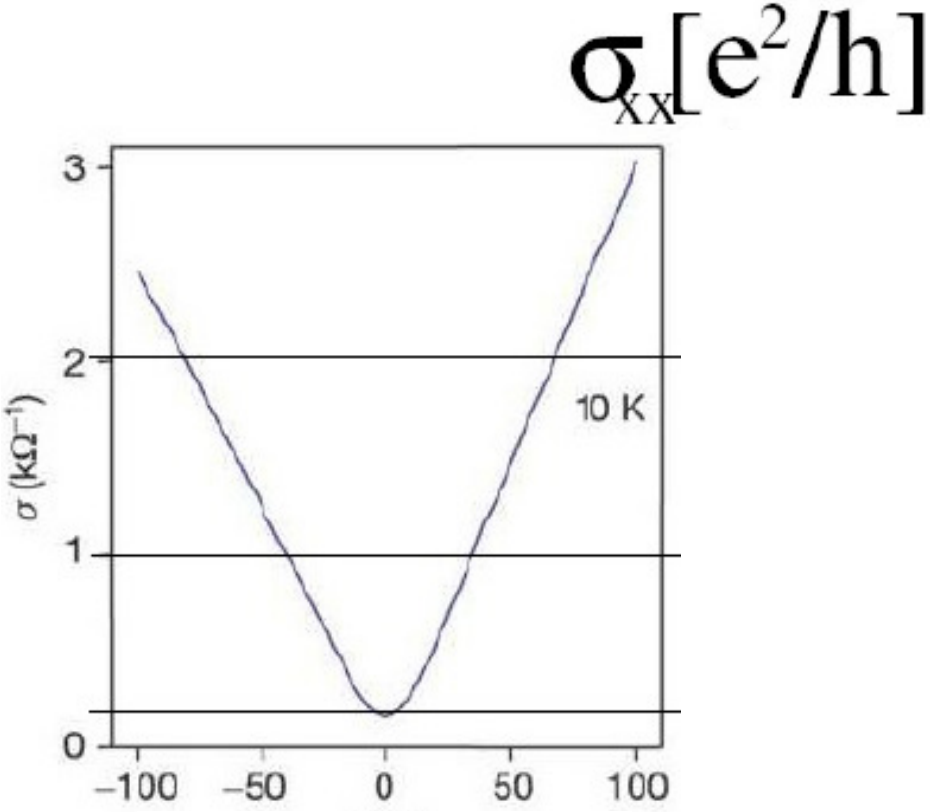
Graphene in many dimensions:

- 3D in graphite crystals
- 2D in a single layer
- 1D in nanotubes
- 0D in fullerenes



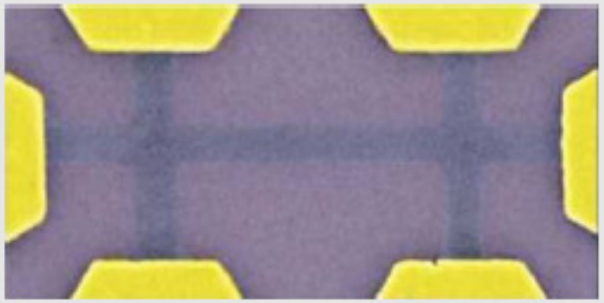
Quantum tunneling and conductivity in Graphene





Electron density

Anomalous QHE in graphene



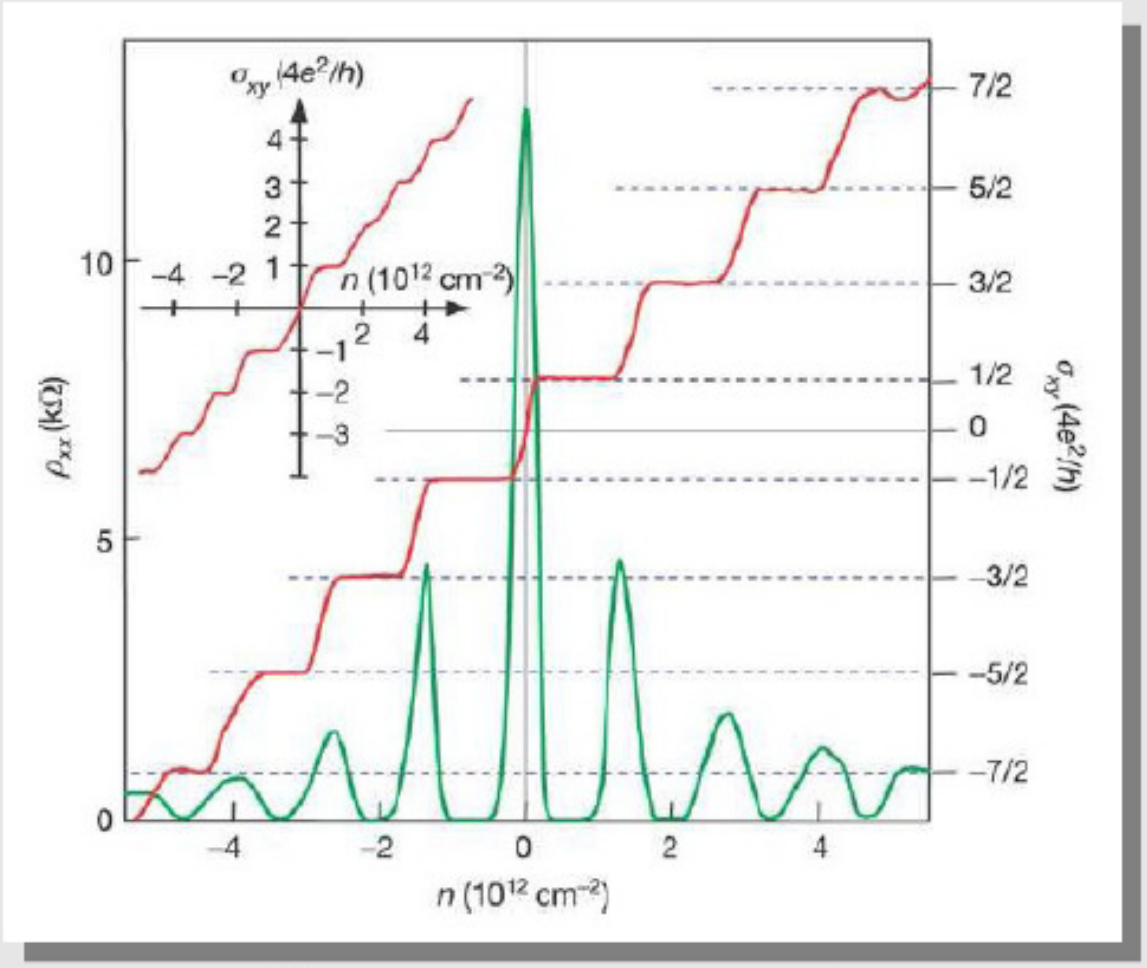
Hall bar, SEM false colors (L=200nm)

QHE in graphene

$$\sigma_{xy} = 4\left(\frac{e^2}{\hbar}\right)\left(n \pm \frac{1}{2}\right)$$

normal QHE

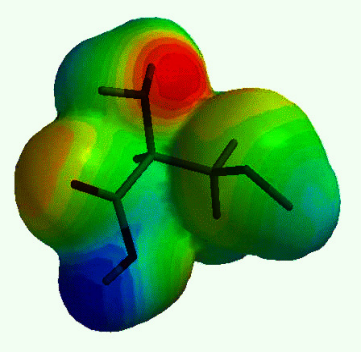
$$\sigma_{xy} = \left(\frac{e^2}{\hbar}\right) n$$



(Novoselov et al., Nature 2005)

Density Functional Theory

The 1998 Nobel Prize in quantum chemistry to Walter Kohn and John A. Pople

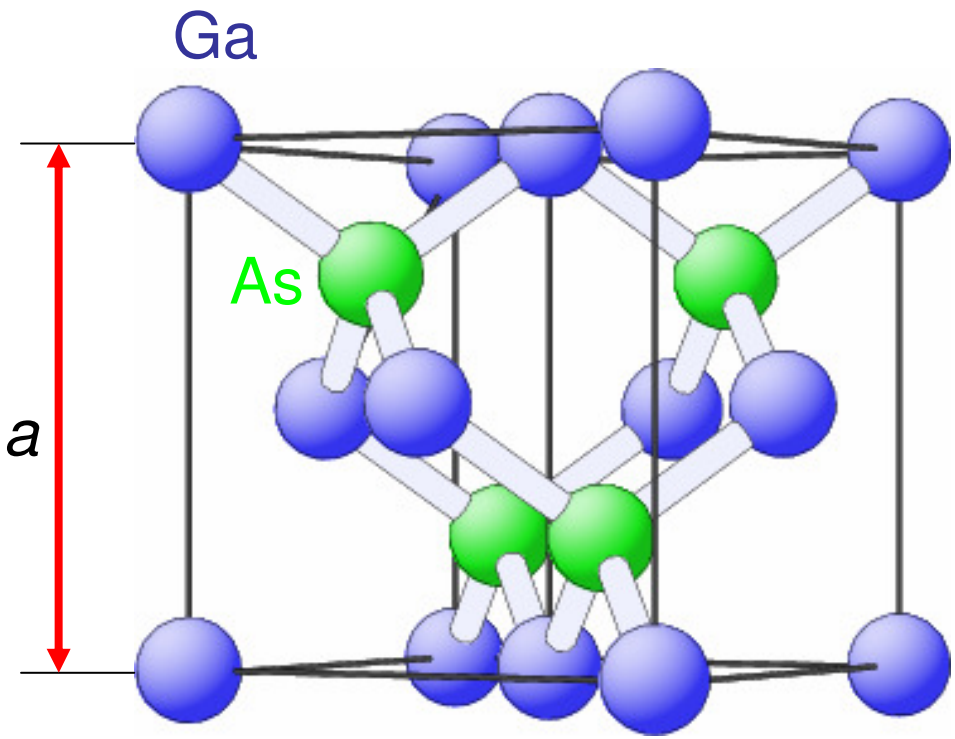


DFT returns an intuitive picture: Density "clouds" $n(\mathbf{r})$

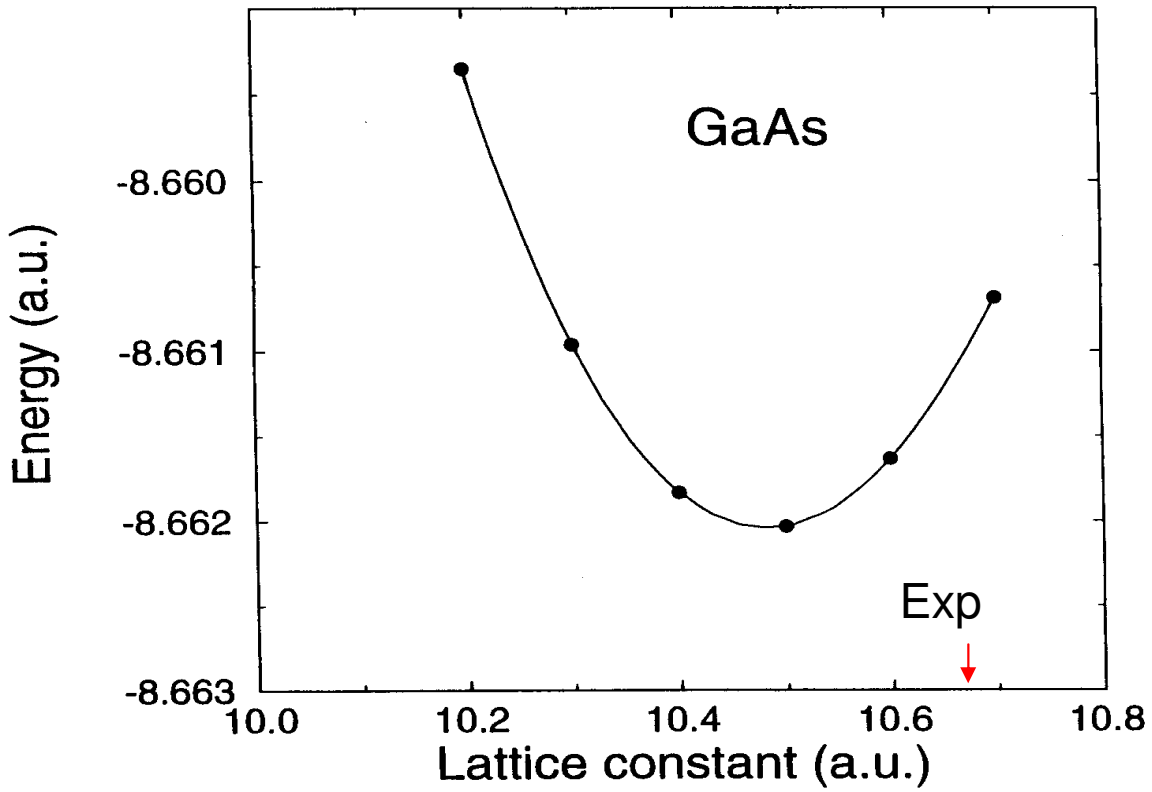
$$n(\mathbf{r}) = N \int d\mathbf{r}_2 \ldots d\mathbf{r}_N \, |\Psi(\mathbf{r}, \mathbf{r}_2, \mathbf{r}_3, \ldots, \mathbf{r}_N)|^2$$

Calculation of a crystal structure

Lattice constant of GaAs



Total energy of GaAs



Protein structure

Joel Ireta[1], Jörg Neugebauer[1,2,3], Matthias Scheffler[1], Arturo Rojo[4], and Marcelo Galván[4]

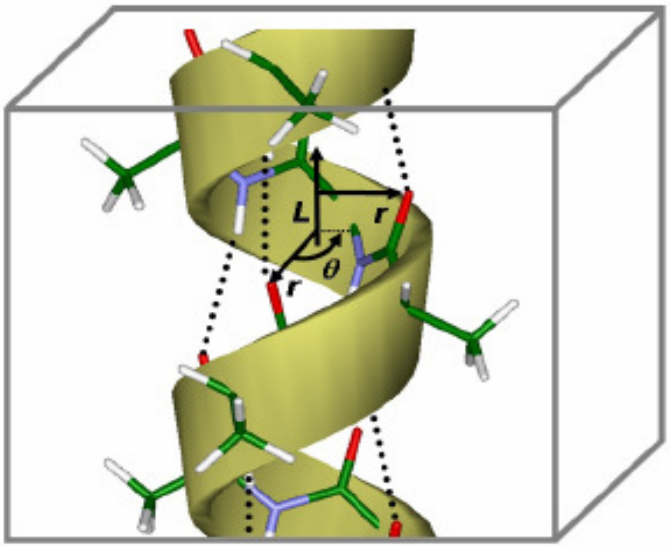


FIG. 1: (color) Schematic geometry of polyalanine in helical conformation inside the employed supercell. Dotted lines mark the hydrogen bonds. Nitrogen atoms are shown in blue, oxygen atoms in red, carbon atoms in green and hydrogen atoms in white. L, r, θ are the helix geometry parameters (length, radius, twist angle), as also described in the text.

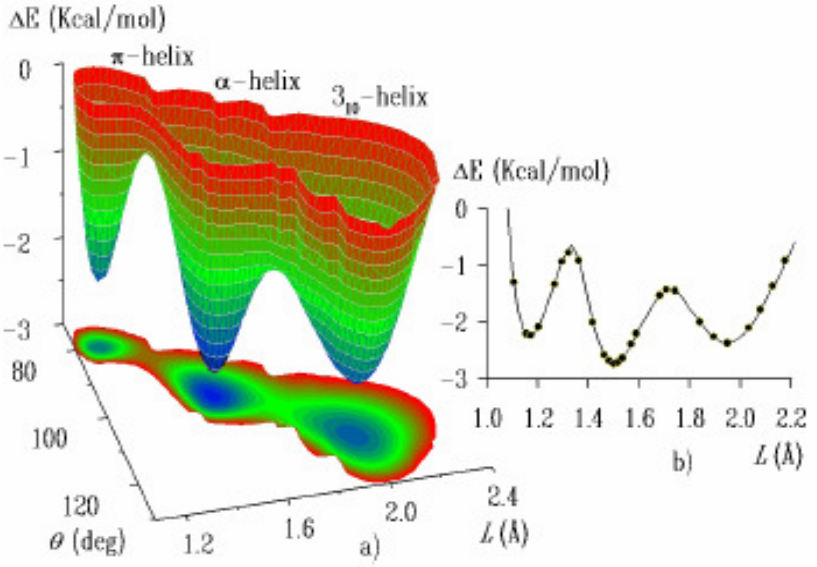
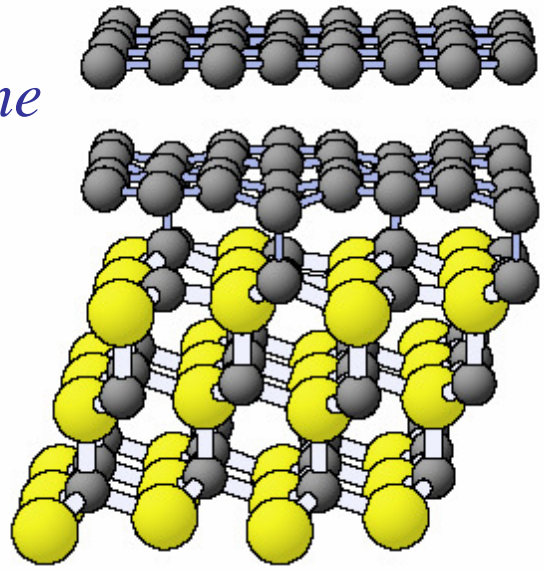


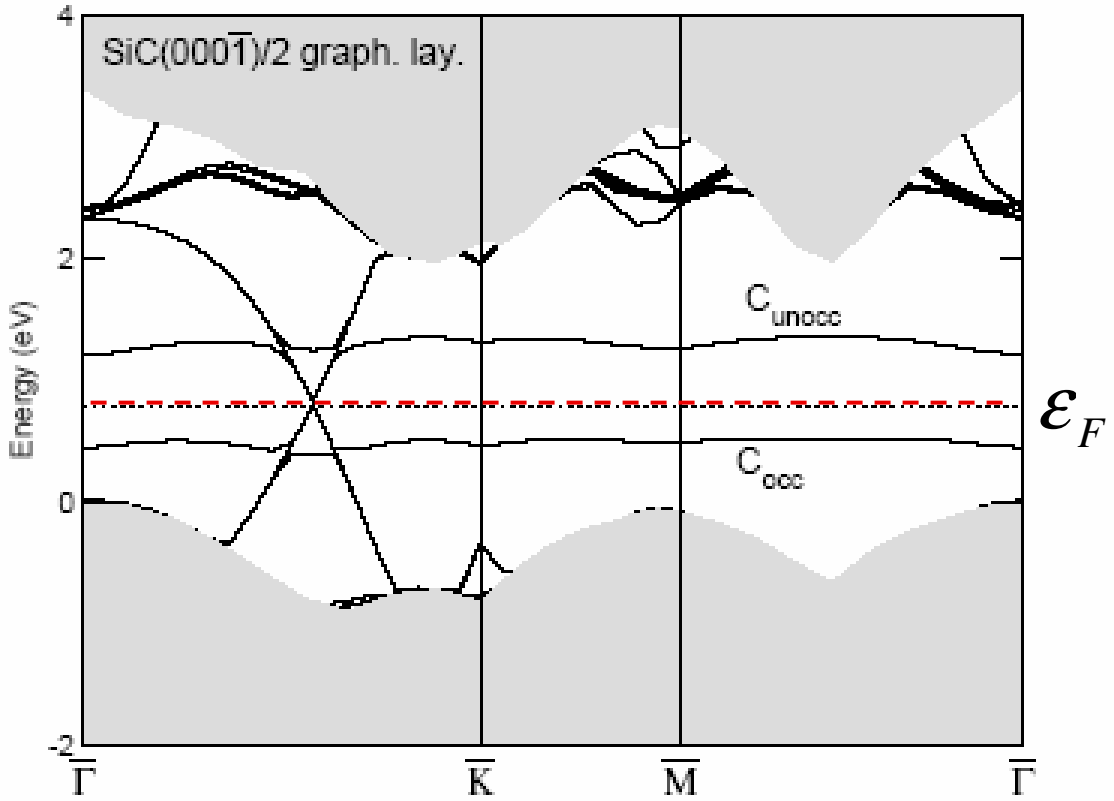
FIG. 2: (color) a) Calculated potential-energy surface as function of the helix length, L, twist angle θ of an infinite polyalanine chain. The helix radius is fully relaxed, as are all other internal parameters of the 10 atoms per peptide unit. b) Minimum energy pathway along (cf. panel a). The dots mark points where actual DFT calculations where performed

Theory-aided design of new materials
Graphene on SiC

Graphene

SiC



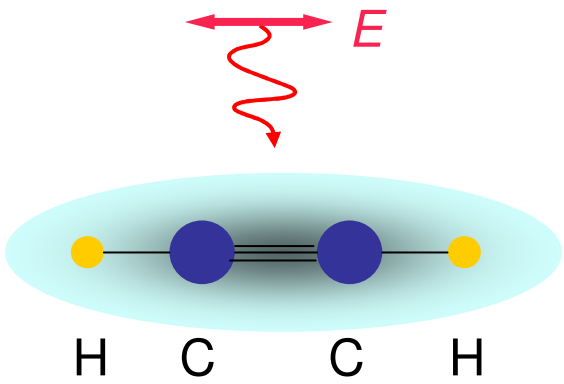


Time dependent processes on electron's time scale

Femtosecond: $1\ fs = 10^{-15}\ s$

Attosecond: $1\,as = 10^{-18}\,s$

Laser excitation of a molecule



Laser excitation of acetylen *(Gross et al)*

$$\hbar\omega = 17\,eV; \quad I_{\max} = 10^{14} W \cdot cm^{-2}; \quad \Delta T = 8\,fs$$

$$H - C \equiv C - H$$