From molecules and clusters of atoms to solid state properties

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UNIVERSITÀ
degli STUDI
di CATANIA

Emergence from complexity

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4 August 1972, Volume 177, Number 4047

SCIENCE

More Is Different

Broken symmetry and the nature of the hierarchical structure of science.

P. W. Anderson

The reductionist hypothesis may still be a topic for controversy among philosophers, but among the great majority of active scientists I think it is accepted

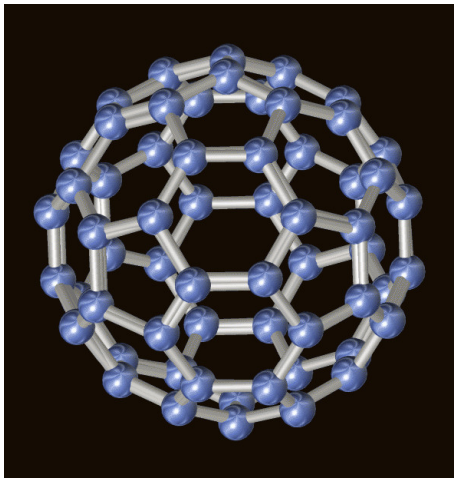
planation of phenomena in terms of known fundamental laws. As always, distinctions of this kind are not unambiguous, but they are clear in most cases. Solid state physics, plasma physics, and perhaps

less relevance they seem to have to the very real problems of the rest of science, much less to those of society.

The constructionist hypothesis breaks down when confronted with the twin difficulties of scale and complexity. The behavior of large and complex aggregates of elementary particles, it turns out, is not to be understood in terms of a simple extrapolation of the properties of a few particles. Instead, at each level of complexity entirely new properties appear, and the understanding of the new behaviors requires research which I think is as fundamental in its nature as any other. That is, it seems to me that one may array the sciences roughly linearly in a hierarchy, according to the idea: The elementary entities of science X obey the laws of science Y.

P. W. Anderson, Science (1972)

sp^2 carbon allotropes: dimensional "diversity"



A. H. Castro Neto *et al.*, Physics World (November 2006); Rev. Mod. Phys. 81, 109 (2009)

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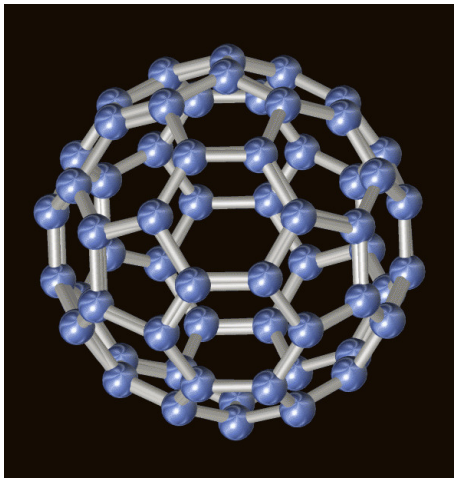

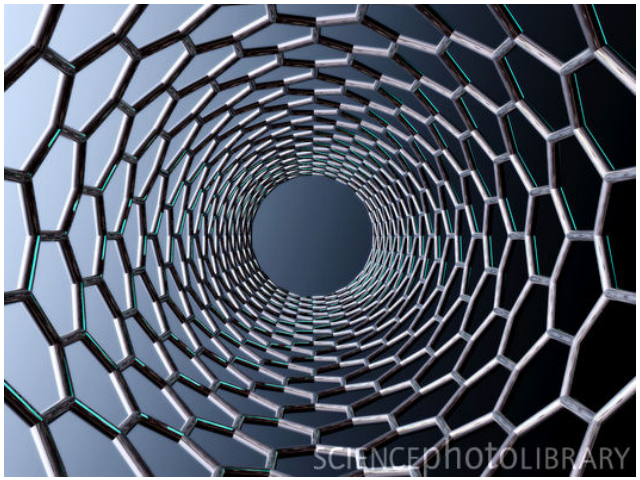

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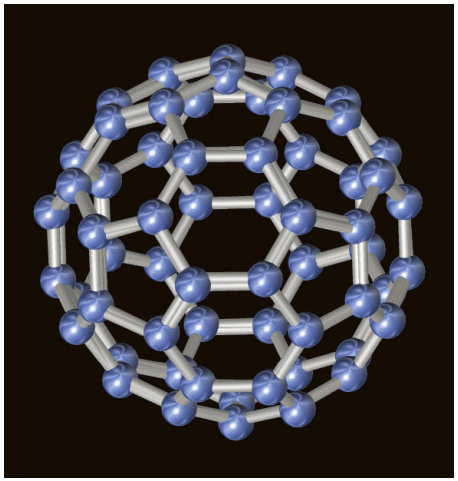

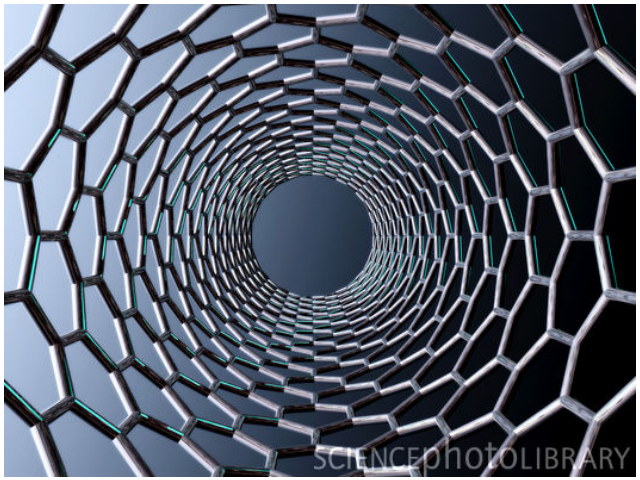

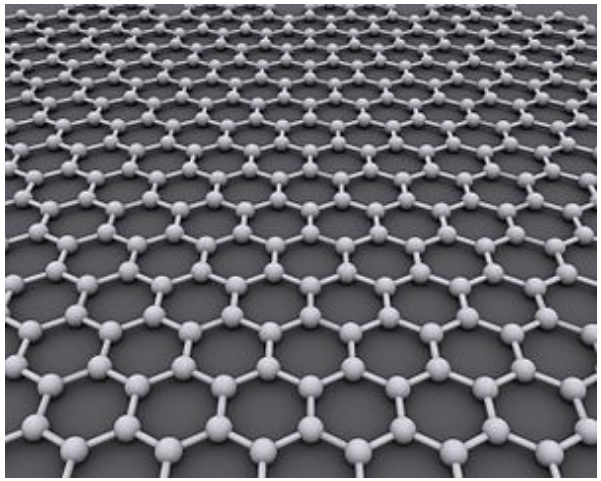

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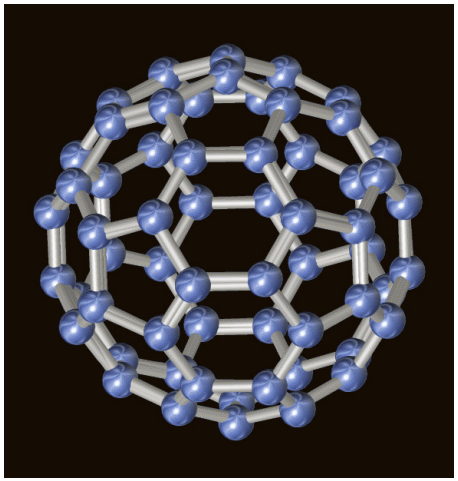
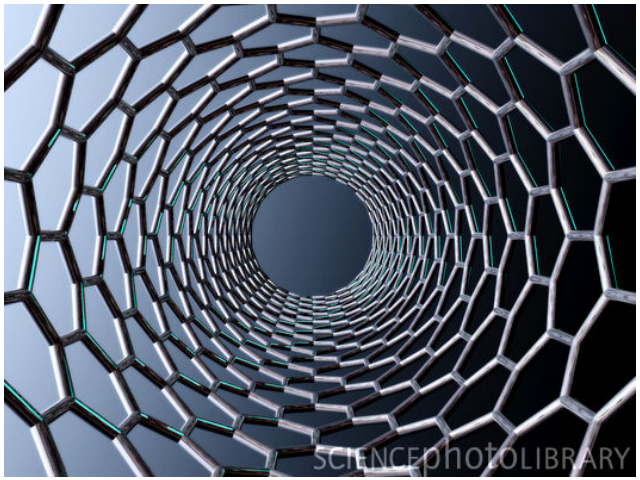
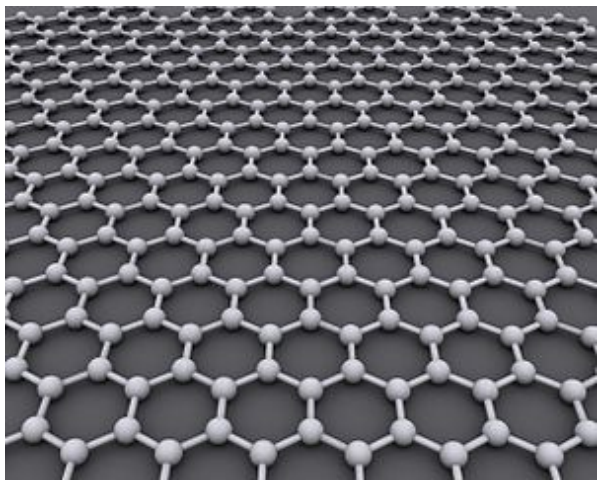
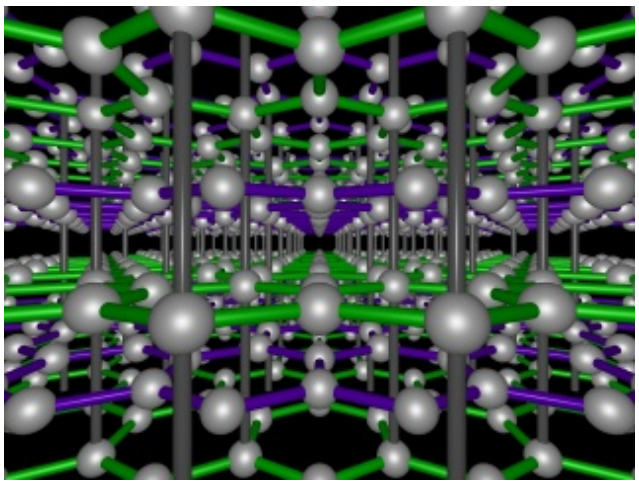


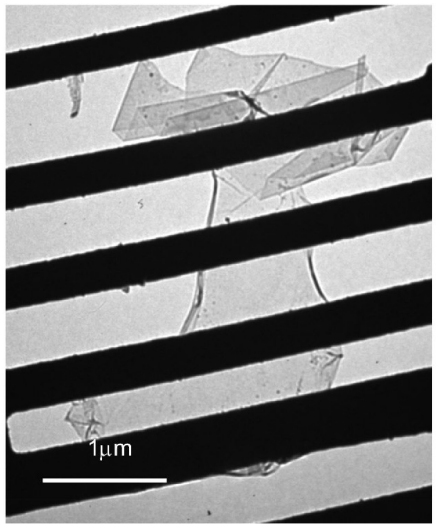


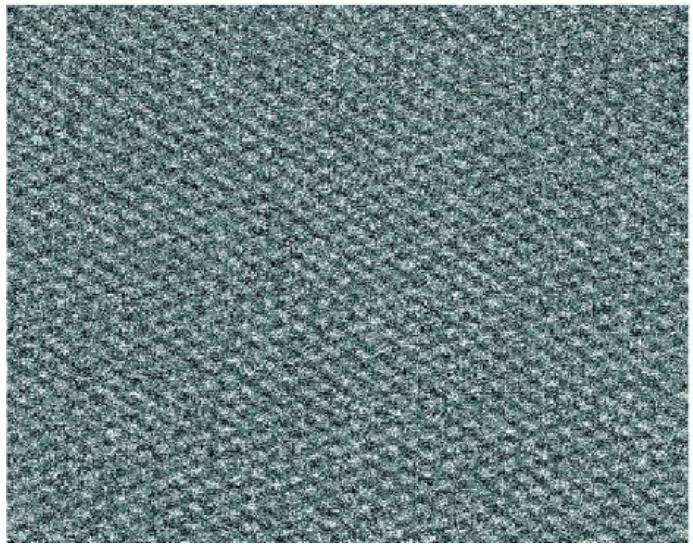




A. H. Castro Neto *et al.*, Physics World (November 2006); Rev. Mod. Phys. 81, 109 (2009)

Synthesis

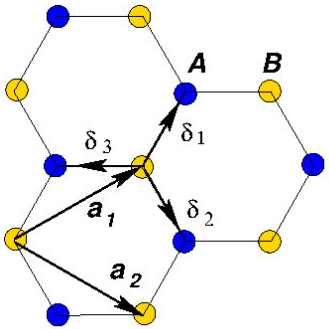


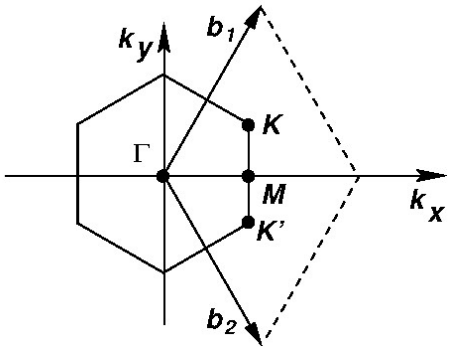


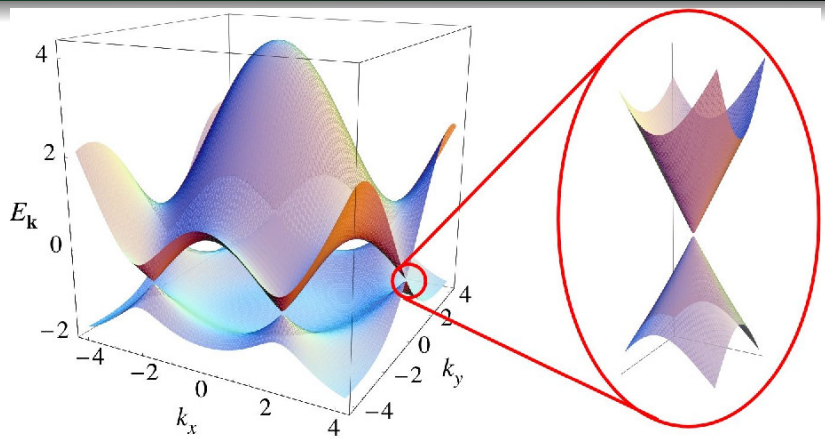
- single layer, one-atom thick
- $L \approx 10\mu$m
- charge mobility $\approx 1.5 \rightarrow 6 \times 10^4$ cm^2/Vs (300 $\rightarrow$ 4 K)

K. S. Novoselov, A. K. Geim, *et al.*, Science **306**, 666 (2004); Meyer *et al.* (2007); Nair *et al.* (2008)

Band structure







- Two inequivalent "Dirac points" at $\mathrm{K}_\pm \equiv \mathrm{K}, \mathrm{K}'$
- $\mathrm{k} = \mathrm{K}_\pm + \mathrm{q}, \qquad E_\pm(\mathrm{q}) = \pm v_\mathrm{F}|\mathrm{q}| + O((q/K)^2)$
- $v_\mathrm{F} = 3ta/2 \approx 1 \times 10^6\ \mathrm{m/s} \approx c/300$

P. R. Wallace, Phys. Rev. **71**, 622 (1947)

- Zero-gap semiconductor: Linear DOS at the Fermi level
- Similarity with nodal superconductors (*e.g.* *d*-wave cuprates)

P. A. Lee, Science **50**, 277 (1997)

Graphene: Mechanical properties

- Exceptional tensile strength of carbon sp^2 compounds
- Graphene can (reversibly) sustain elastic strain $\varepsilon \lesssim 20$ %
- Record breaking strength (~ 40 N/m) and Young modulus (~ 1.0 TPa)

C. Lee *et al.*, Science **321**, 385 (2008)

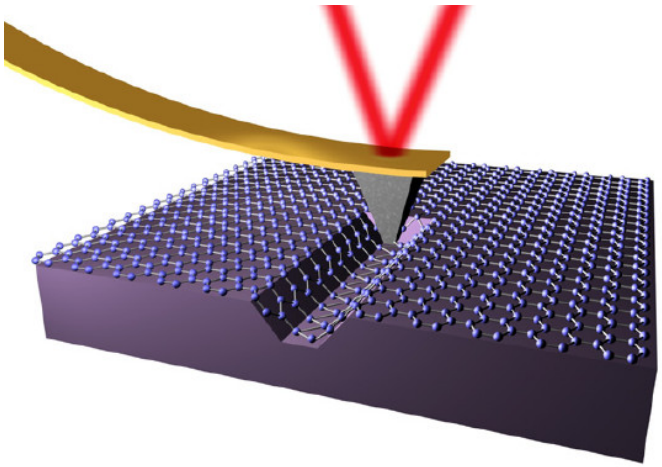
- *Ab initio* studies of uniaxial strain effects

E. Cadelano *et al.*, Phys. Rev. Lett. **102**, 235502 (2009)

- Origami nanodevices and straintronics

V. M. Pereira and A. H. Castro Neto, Phys. Rev. Lett. **103**, 046801 (2009)

Strained graphene: *how to*



- AFM nano-indentation on suspended graphene (SiO_2)

C. Lee *et al.*, Science 321, 385 (2008)

- graphene on flexible substrate

K. S. Kim *et al.*, Nature 457, 706 (2009).

- graphene bubbles ($R \sim 4\ \mu$m)

R. Huang, Nature Nanotech. 6, 537 (2011)

J. Zabel *et al.*, Nano Lett. 12, 617 (2012)

- gate-controlled strain

M. M. Fogler *et al.*, PRL 101, 226804 (2008)

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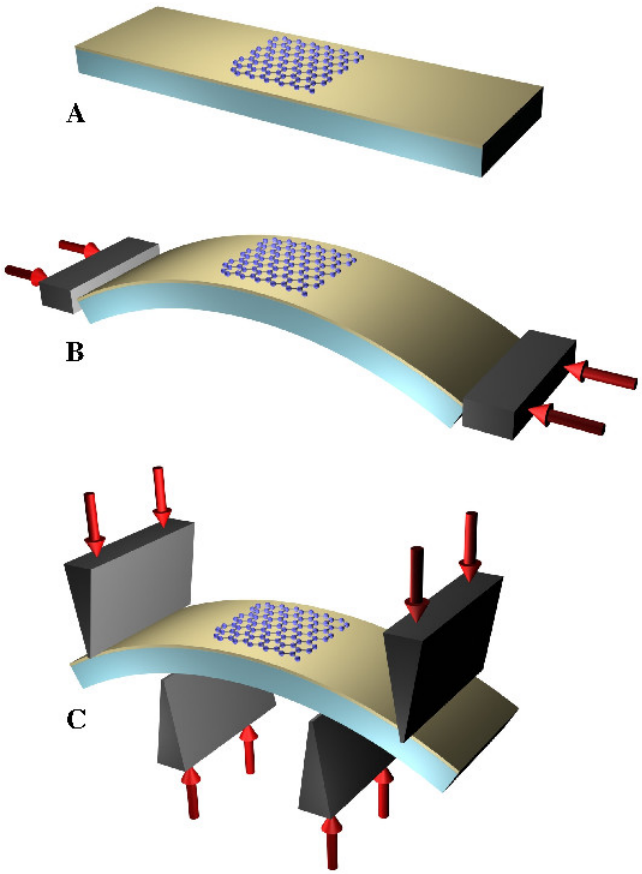

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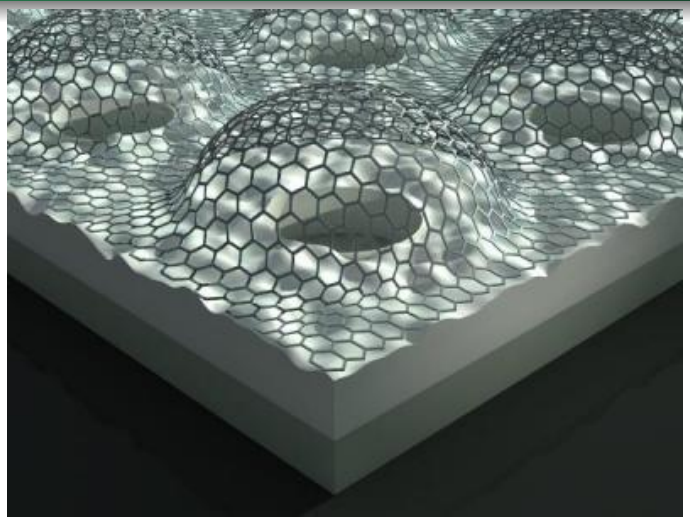

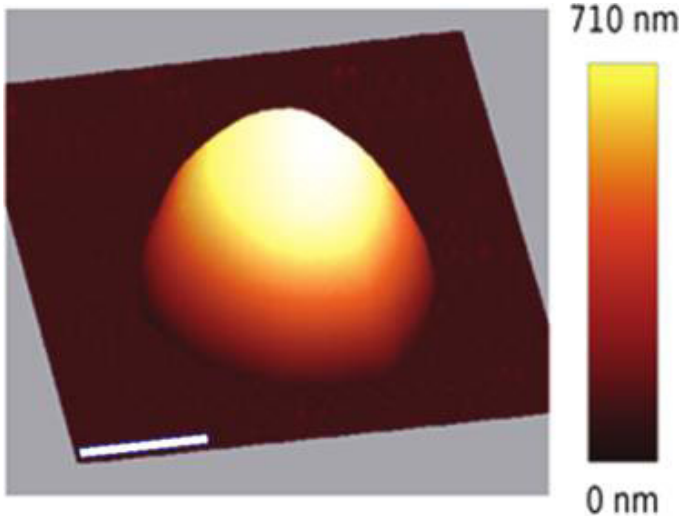

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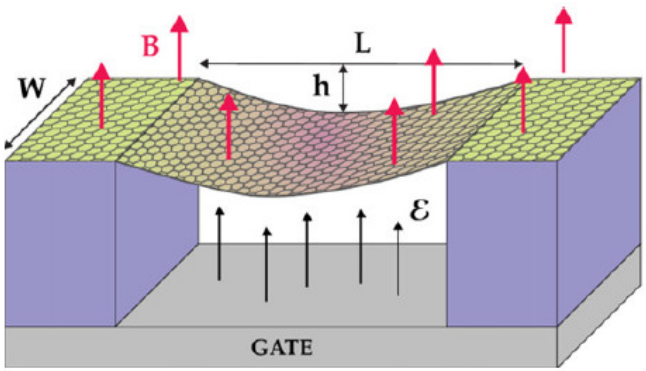

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Correlations in π-electron molecular systems

- RPA+LFC in ethylene

M. Baldo and R. Pucci, JChemPhys (1977)

M. Baldo, R. Pucci, and P. Tomasello, JChemPhys (1979)

- Electronic structure of linear polyacenes

M. Baldo, A. Grassi, R. Pucci, and P. Tomasello, JChemPhys (1982)

- RPA+LCF in benzene

R. Pucci, P. Baeri, M. Baldo, R. Parisi, and P. Tomasello, MolPhys (1980)

- SCF-RPA in benzene and naphtalene

M. Baldo, A. Grassi, R. Pucci, and P. Tomasello, ChemPhysLett (1981)

- SCF-RPA in linear polyenes chains

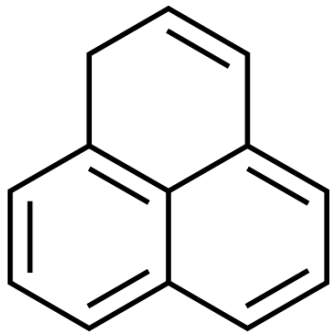
M. Baldo, R. Pucci, and P. Tomasello, IntJQuantChem (1983)

One Ring to rule them all . . .

Benzene, C_6H_6

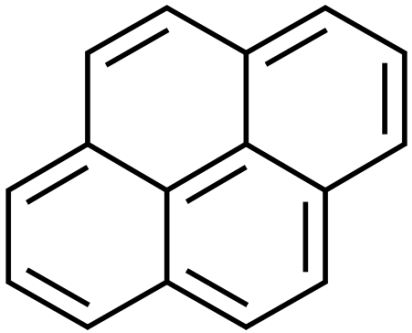
One Ring to rule them all . . .

Phenalene, $C_{13}H_{10}$



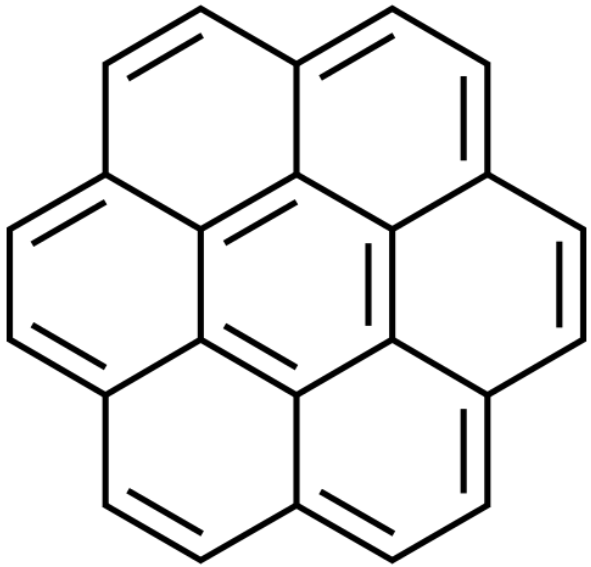
One Ring to rule them all . . .

Pyrene, $C_{16}H_{10}$



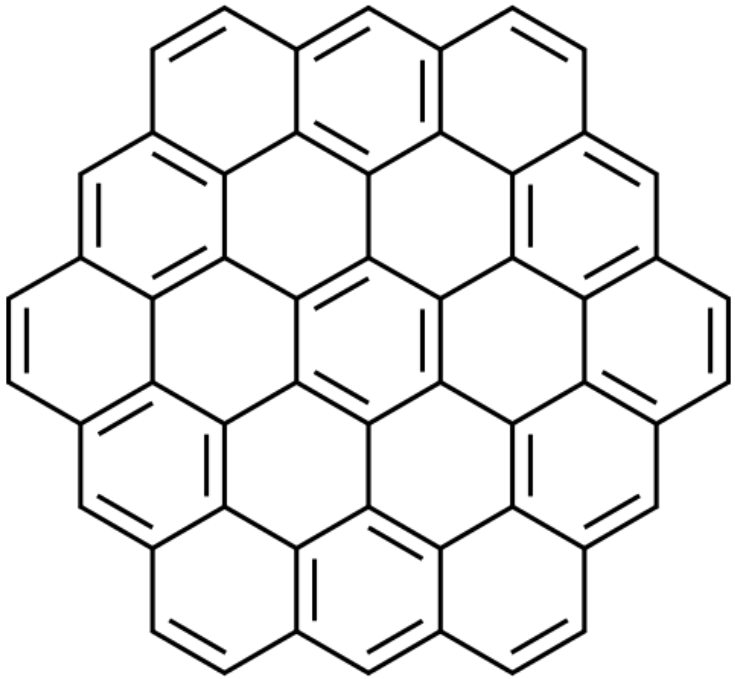
One Ring to rule them all ...

Coronene, $C_{24}H_{12}$



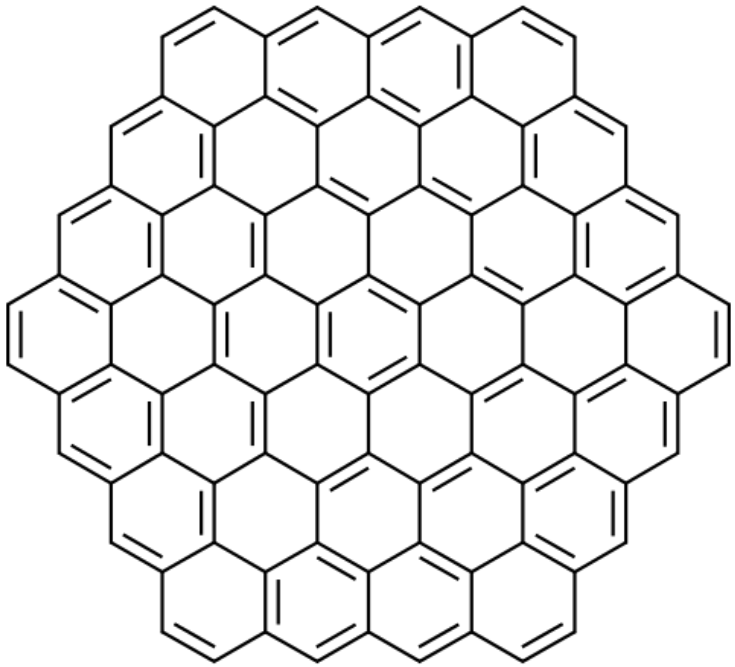
One Ring to rule them all ...

Circumcoronene, $C_{54}H_{18}$



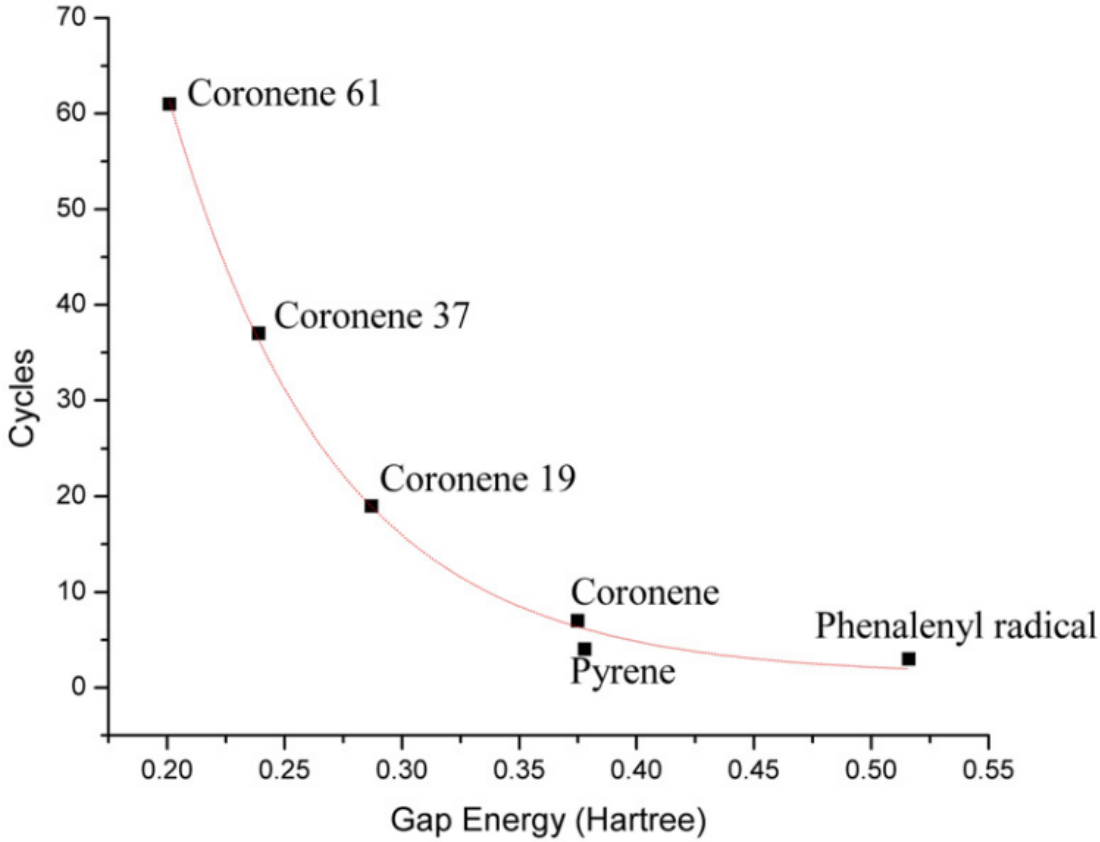
One Ring to rule them all ...

Circumcircumcoronene, $C_{96}H_{24}$



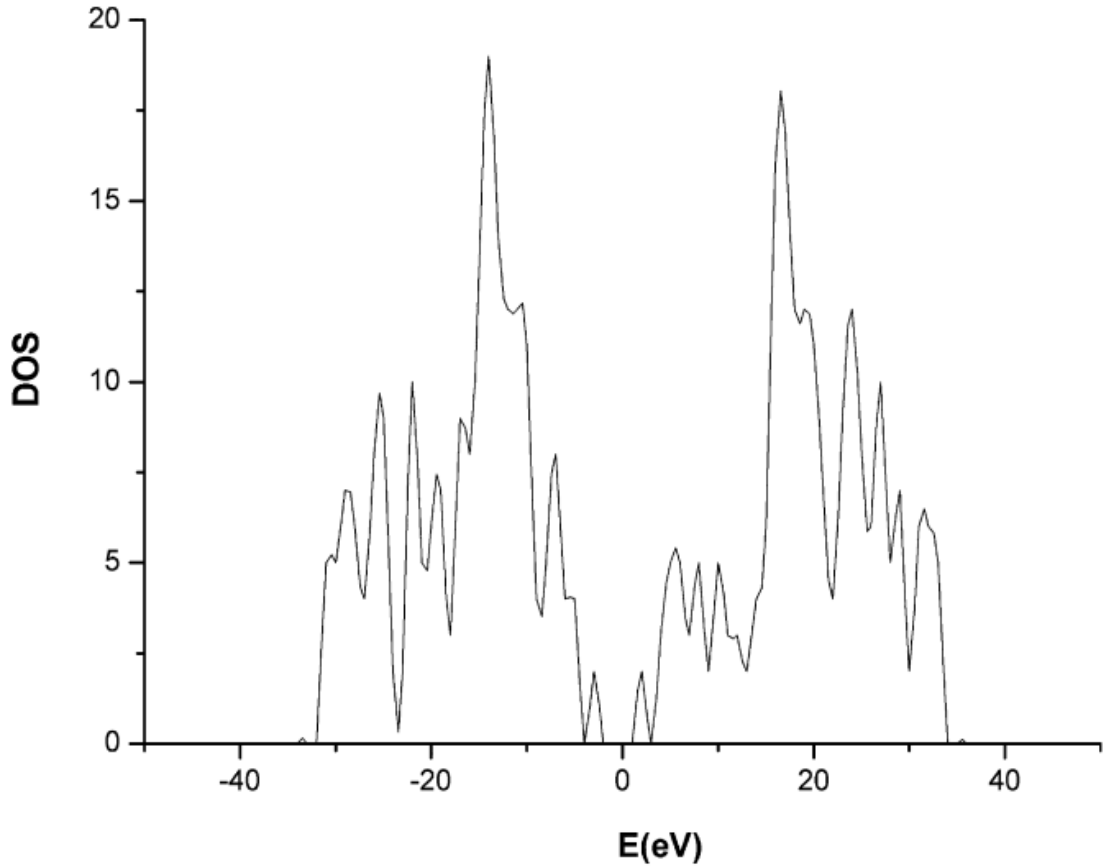
From molecular HOMO-LUMO to solid-state gap

- HOMO-LUMO difference (gap energy) from HF+MP2 calculations



DOS

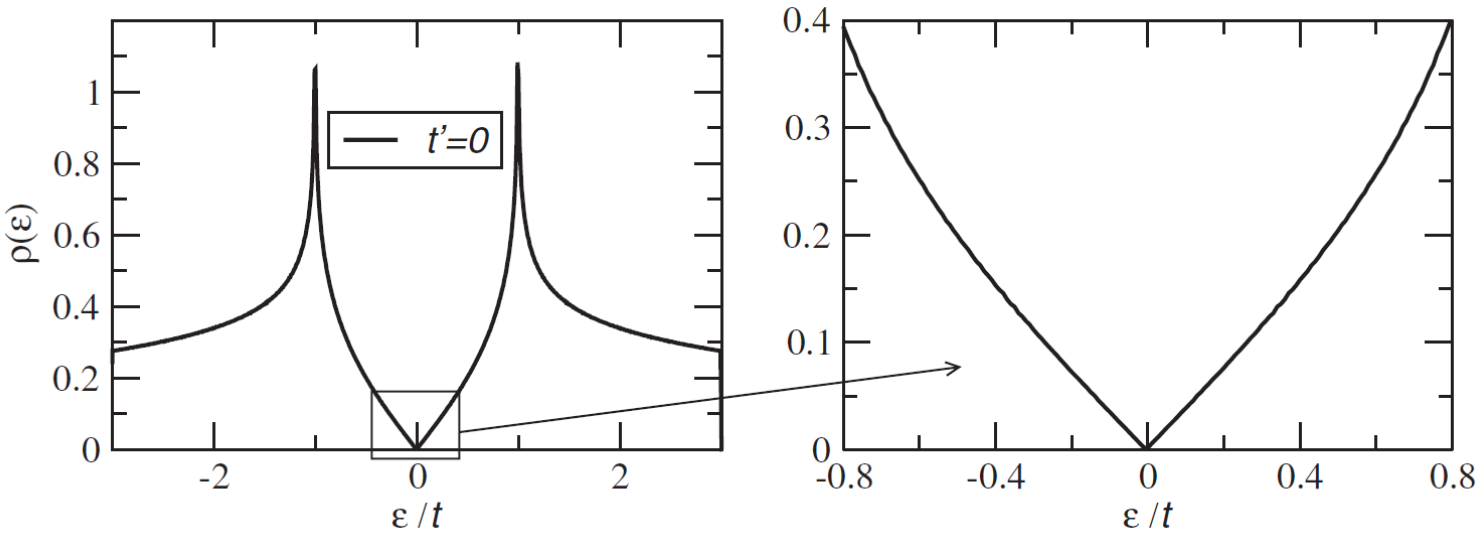
- DOS for coronene 37 from HF+MP2 calculations



G. Forte, A. Grassi, G.M. Lombardo, A. La Magna, GGNA, R. Pucci, R. Vilardi, PLA (2008)

DOS

- DOS for solid state graphene (tight-binding calculations)



A. H. Castro-Neto *et al.*, RMP (2009)

Back to atoms: LDOS at a single impurity in graphene

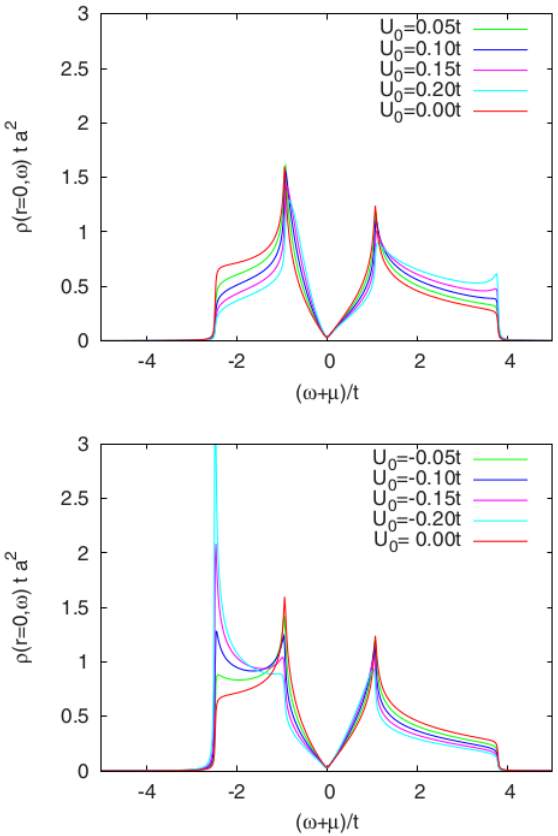
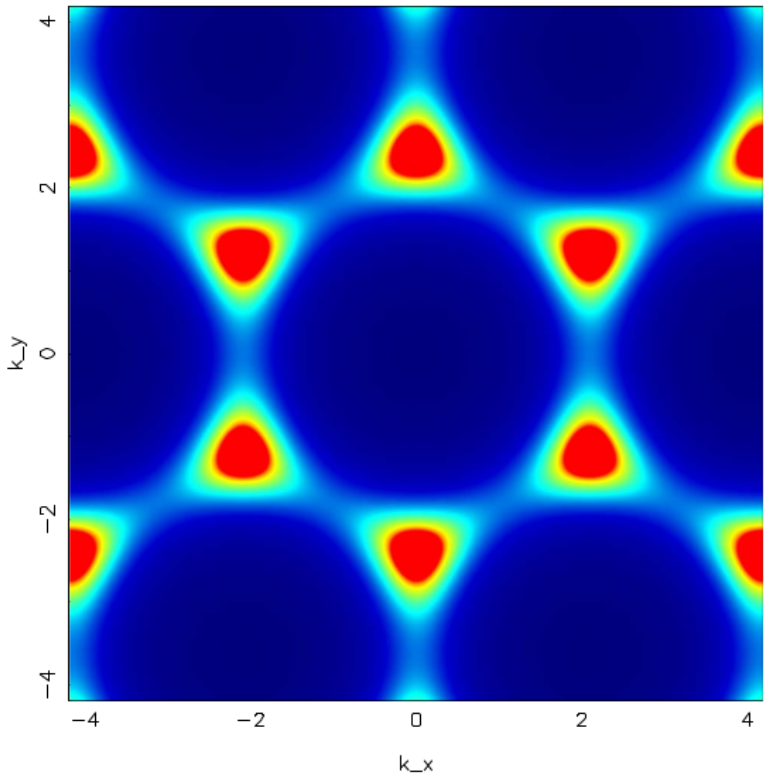


FIG. 2. (Color online) Local density of states $\rho(\mathbf{x}=\mathbf{0},\omega)$, Eq. (19), on a sitelike impurity located at $\mathbf{x}=\mathbf{0}$. Top panel shows the LDOS for $U_0/t=-0.05$, -0.10, -0.15, and -0.20. Bottom panel shows the LDOS for $U_0/t=0.05$, 0.10, 0.15, and 0.20. In both panels, we also show the LDOS in the unperturbed case ($U_0/t=0$).



F.M.D. Pellegrino, GGNA, R. Pucci, PRB (2009)

Ad altiora!