

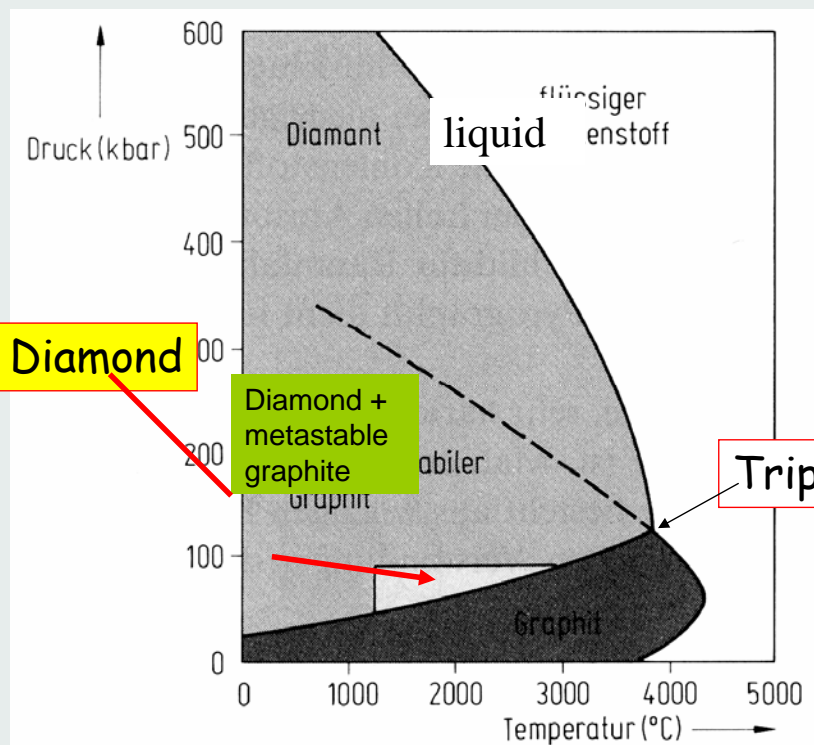
Carbons

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Carbon - Phase Diagram



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Tetrels - Phase Diagrams

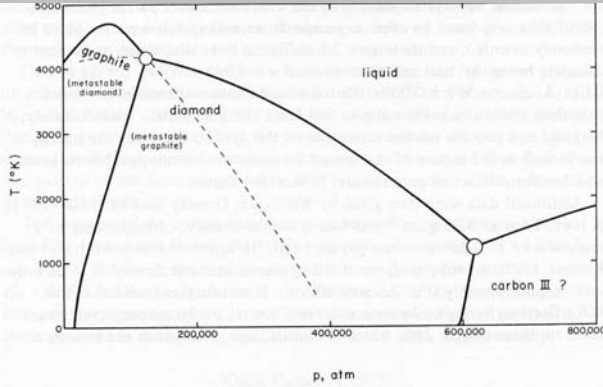
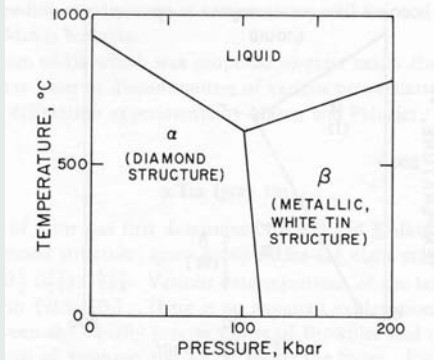
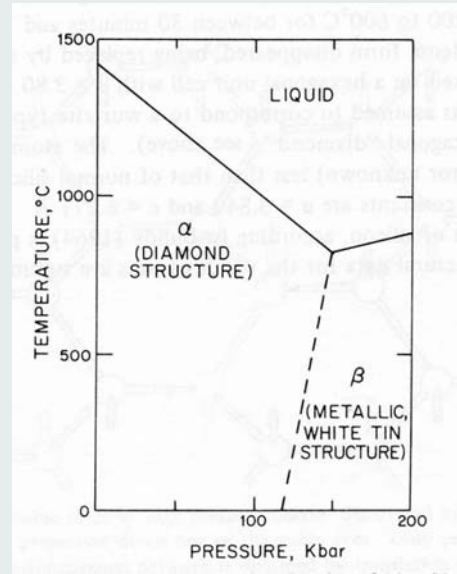


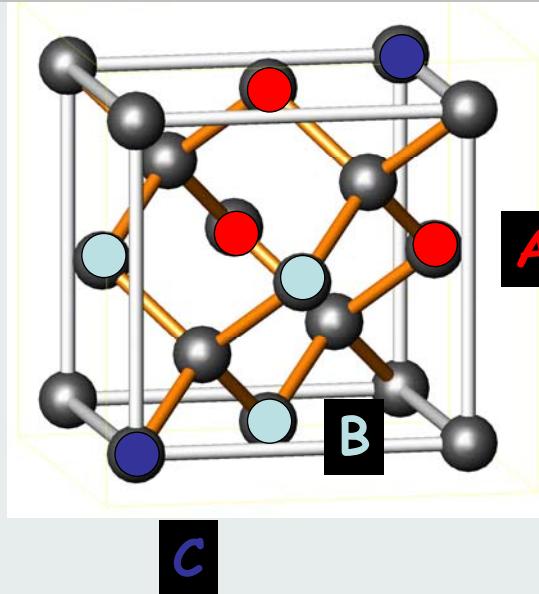
Fig. 6-8. The phase diagram of carbon (after Bundy, 1962).



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Cubic Diamond



1.54 \AA
 $\Delta H_B = 348 \text{ kJmol}^{-1}$

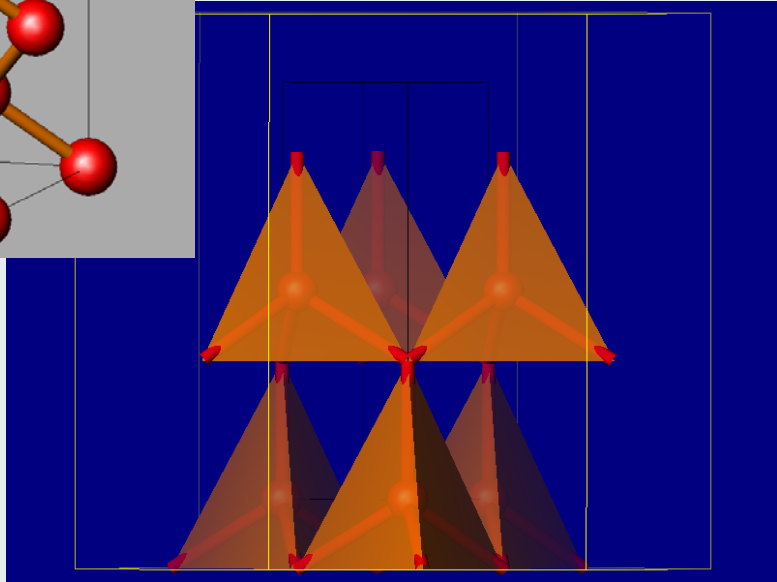
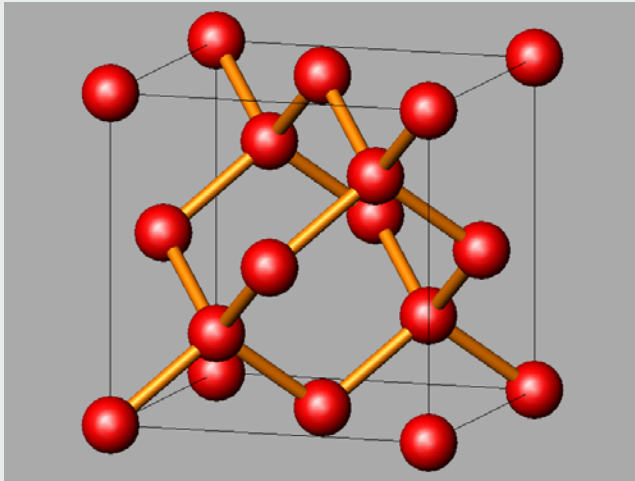
at 1 bar, 25°C metastable; 1500°C: $C_{\text{Diamant}} \rightarrow C_{\text{Graphit}}$

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Diamond

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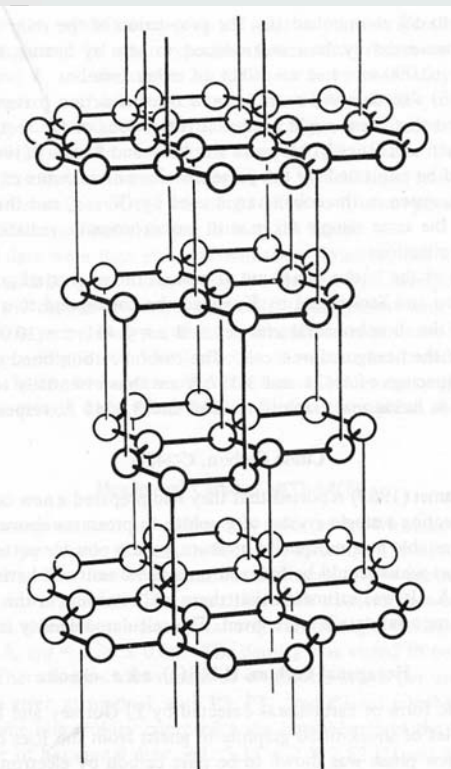


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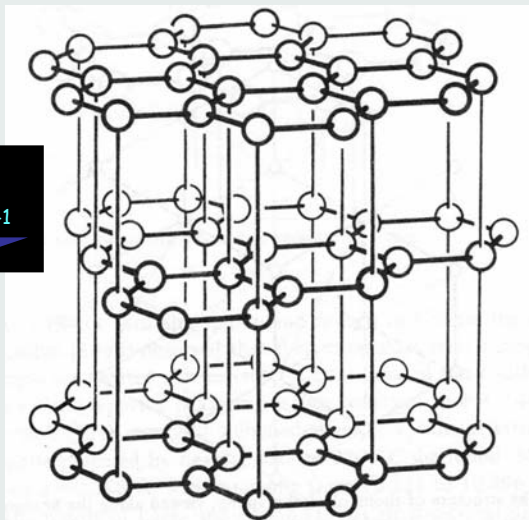


Hexagonal and Rhomboedral Graphite



conductivity: $10^4 \Omega^{-1} \text{cm}^{-1}$

≈ 1
 $\Omega^{-1} \text{cm}^{-1}$

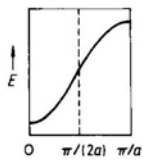
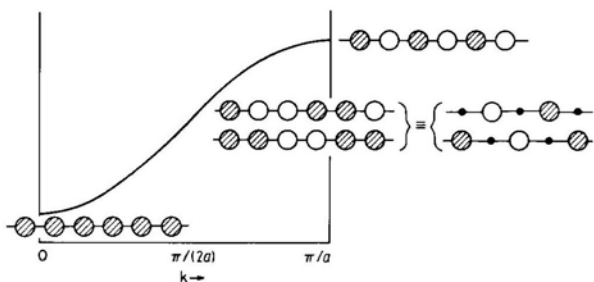
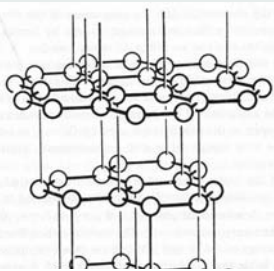


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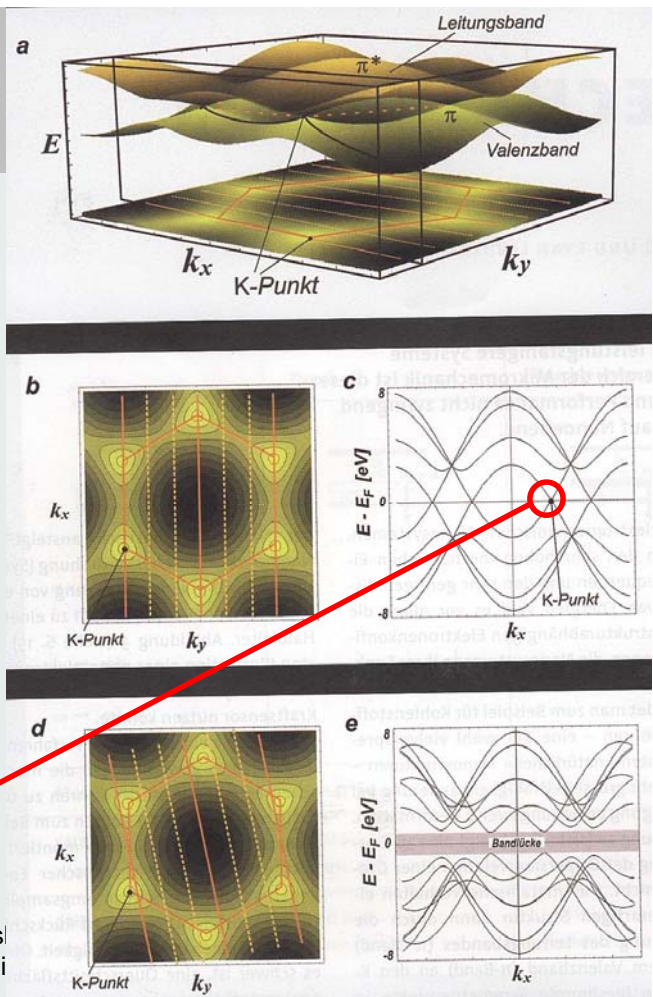


Electronic Conductivity of Graphite

LEGIUM HELVETICUM

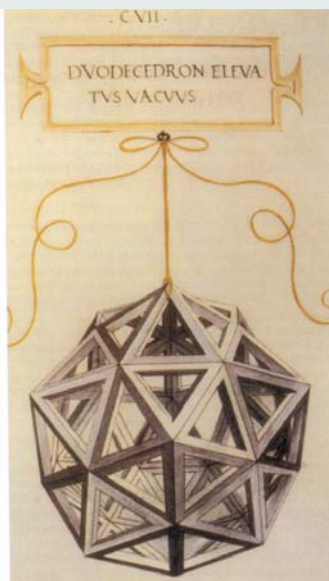


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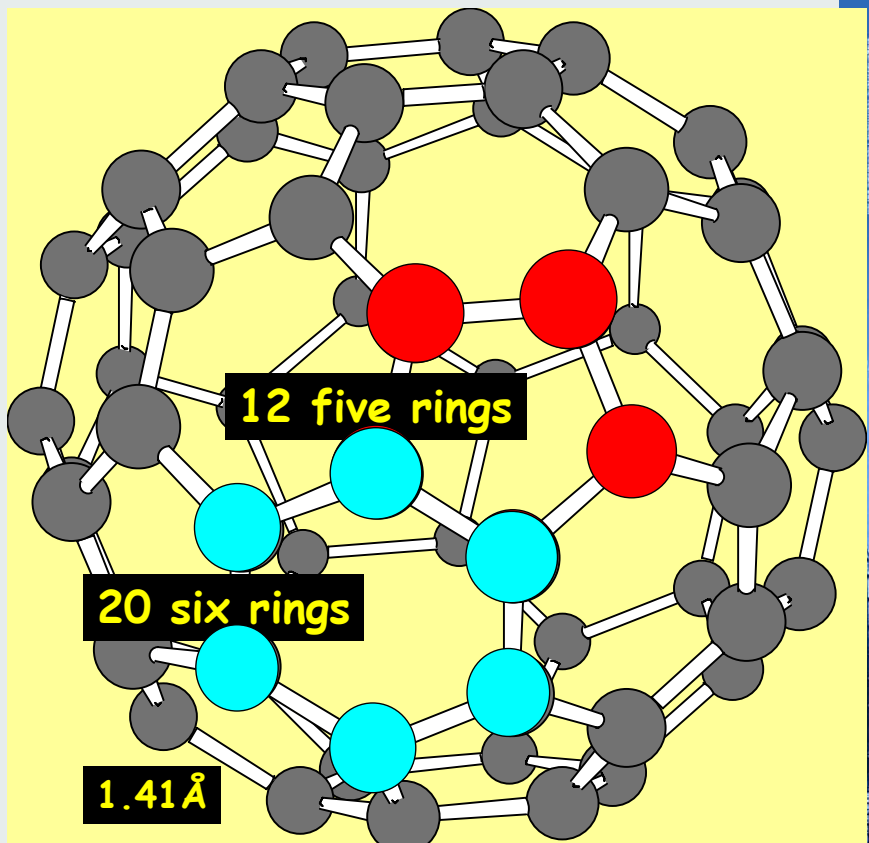
Buckminster-Fullerenes

60 Corners



Ein Kantenstern von Leonardo da Vinci

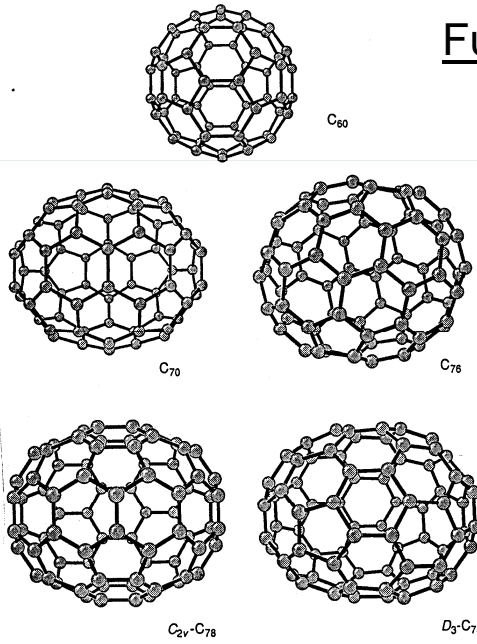
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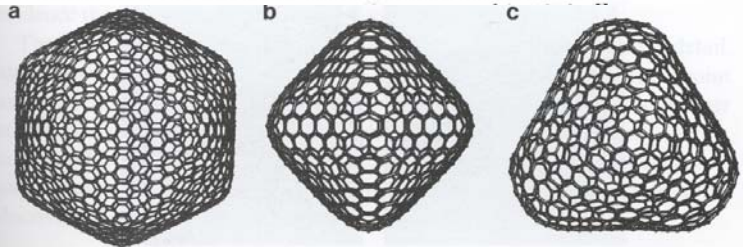
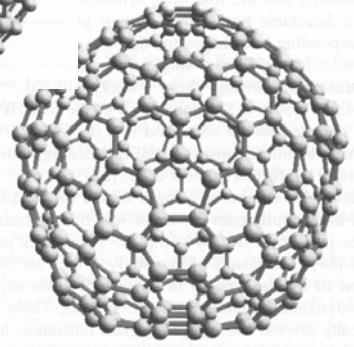
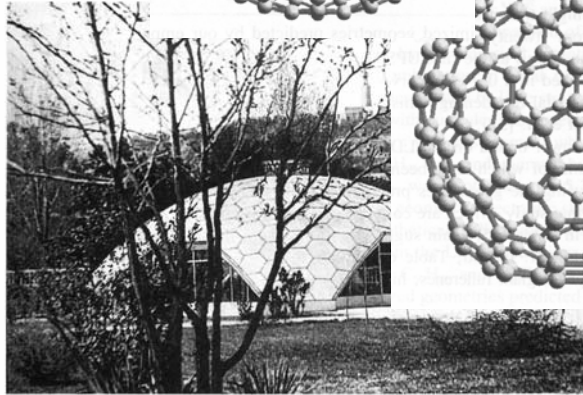
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Fullerenes



Fullerene structures as elucidated by ^{13}C NMR spectroscopy.



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transformation, etc.

C-Fullerene to Diamond

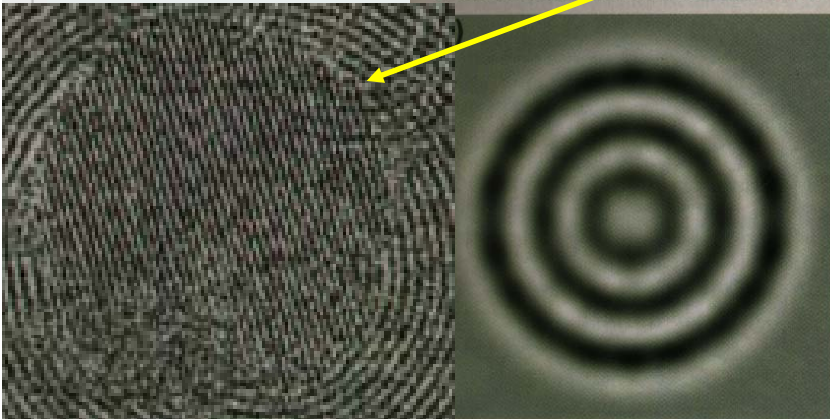
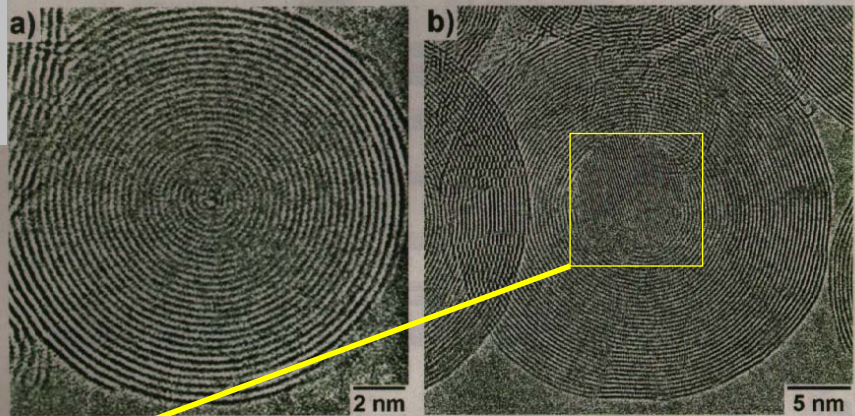


Abb. 2. a) Hochauflösende transmissionselektronenmikroskopische (HRTEM)-Aufnahme einer Kohlenstoffzwiebel. b) HRTEM-Abbildung einer elektronenbestrahlten Kohlenstoffzwiebel mit Diamantkern. (Bild: Dr. F. Banhart/MPI für Metallforschung, Stuttgart). c) HRTEM-Simulation und d) schematische Darstellung einer Kohlenstoffzwiebel. (Bild: Dr. M. Terrones/University of Sussex, U.K.)

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Fullerenes

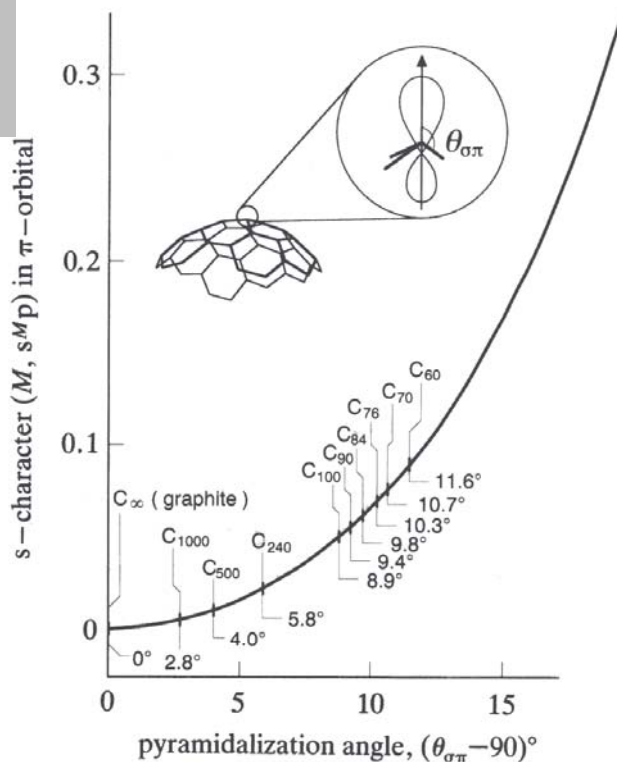


Figure 4. Rehybridization as a function of pyramidalization angle. The π -orbital axis vector (POAV approximation), is defined as that vector which makes equal angles to the three σ -bonds at a conjugated carbon atom (Haddon 1988). The common angle to the three σ -bonds (which are assumed to lie along the internuclear axes), is denoted $\theta_{\sigma\pi}$. The average pyramidalization angle $[(\bar{\theta}_{\sigma\pi} - 90)^\circ]$ shown for representative fullerenes (C_n), was obtained from eqn (2) of Haddon *et al.* (1986b) for $n > 60$.



Fullerene Isomers

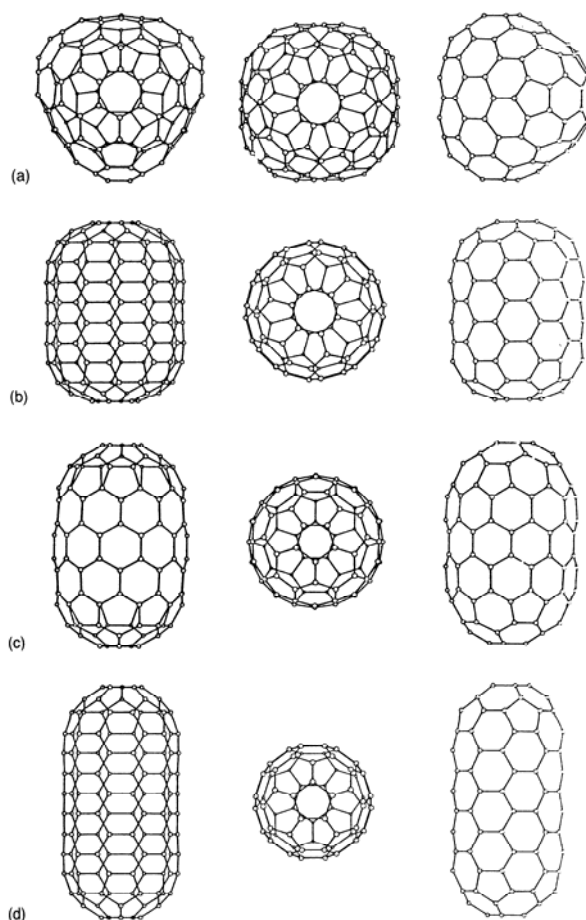
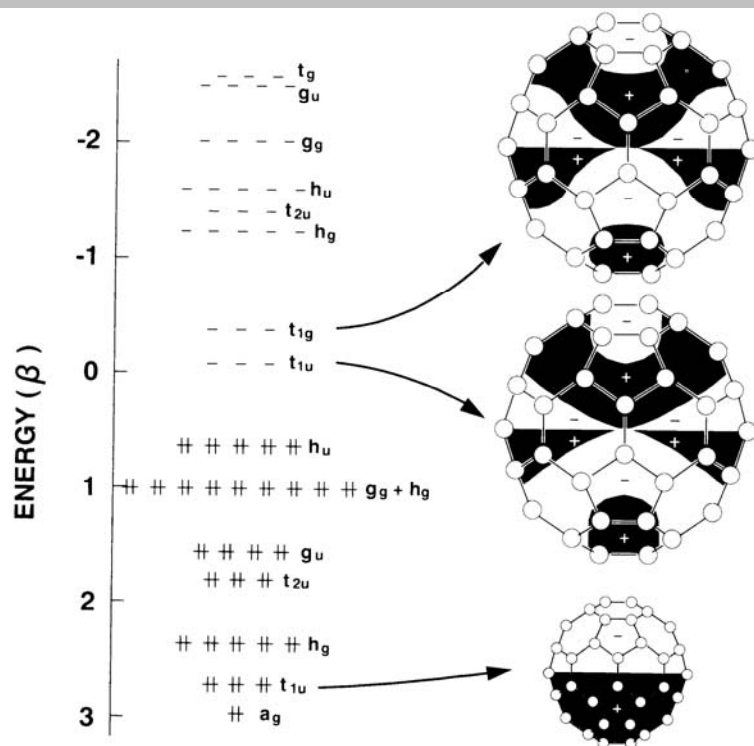


Figure 5.4 Equilibrium geometries of four isomers of C_{120} as predicted by the STO-3G/SCF level of theory: (a) T_d , (b) D_{6d} , (c) D_{3d} SF, (d) D_{3d} VF.

Fullerene Molecular Orbitals



Fullerene
Superconductors

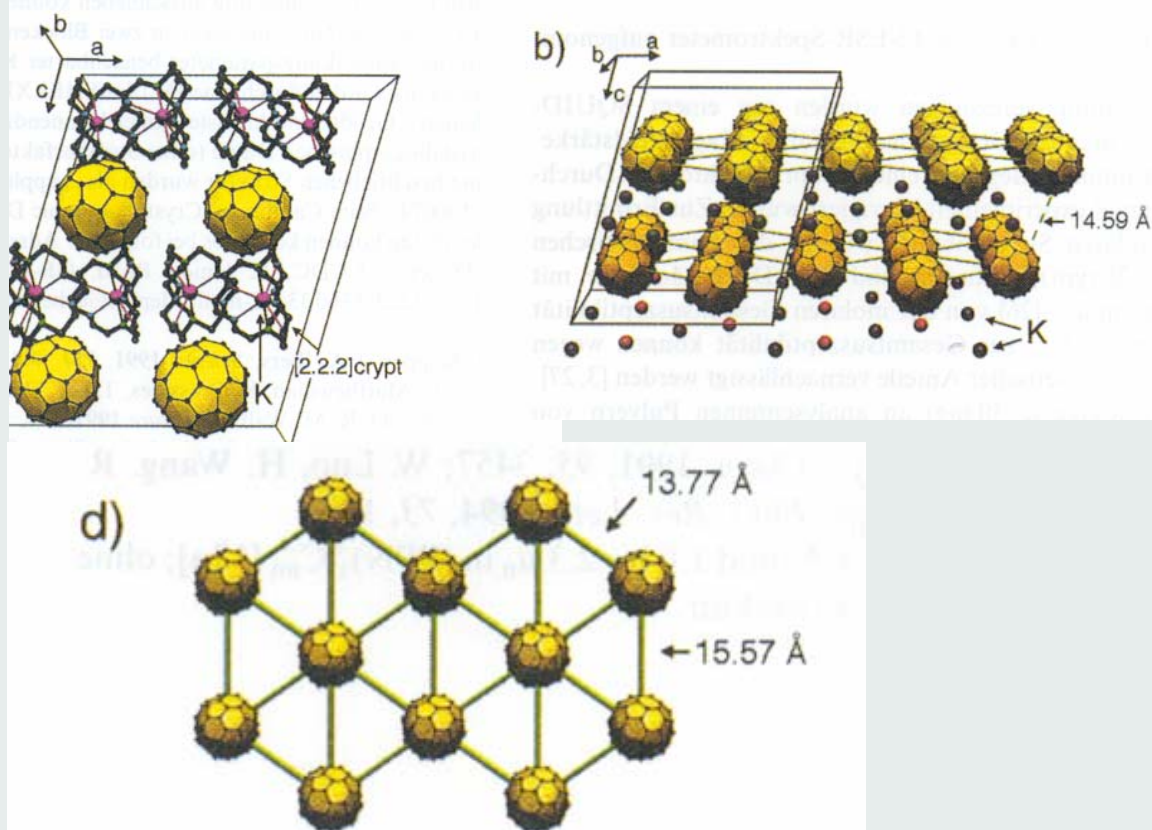
M_3C_{60}

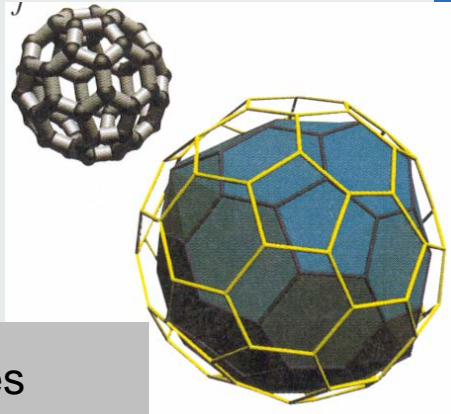
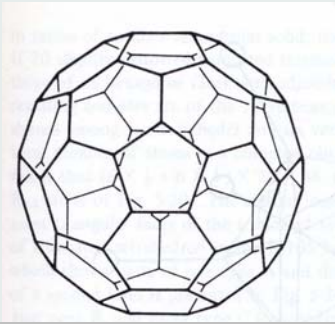
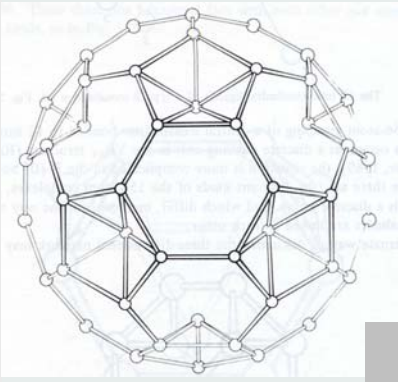
$M=K, Rb$

$T_c(\text{max}) \sim 40K$

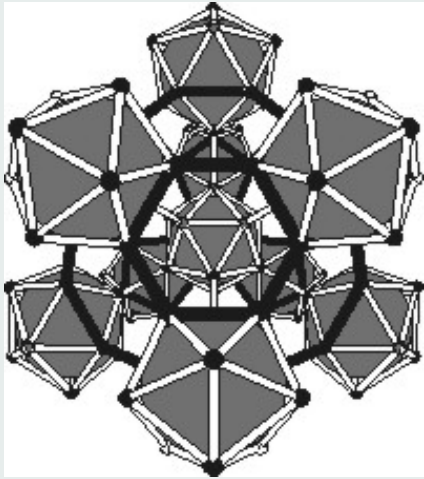
1. Hückel molecular orbital (HMO) energy levels of C_{60} together with one component of the triply degenerate t_{1u} and t_{1g} sets of molecular orbitals.

Fullerene Compounds

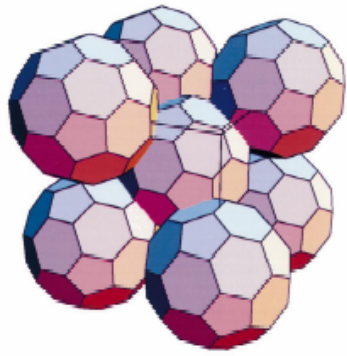
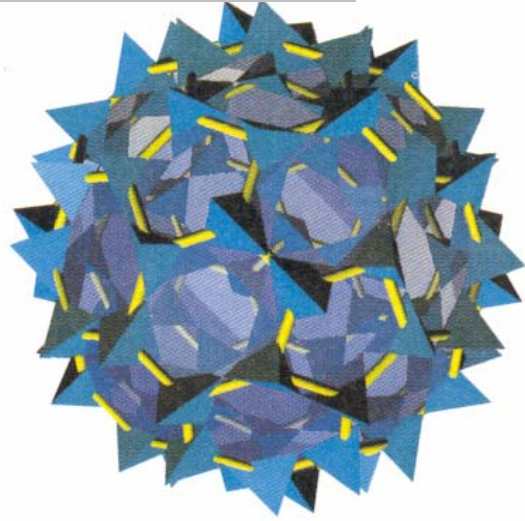




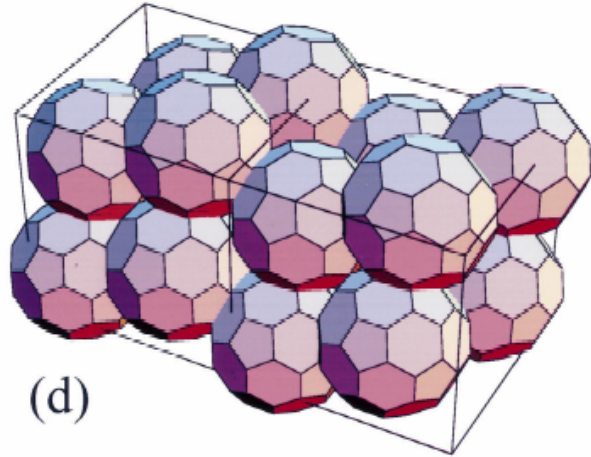
Metal Fullerenes



R. Nes
Nan



(a)



(d)



(b)



(c)

Fig. 2. The structures of two cubic Fibonacci approximants with Bergman clusters (BC) shown as solid soccer balls: (a) b.c.c. packing of BC in the crystal structure of $1/1-(Al,Zn)_3Mg_2$; the connection of Bergman clusters as found in the $1/1$ - and $2/1$ -approximant: (b) clusters along twofold axes are connected via common edges (b bonds) and (c) along threefold axes via common hexagon faces (c bonds); (d) the rhombohedral packing of BCs at the vertices of prolate and oblate rhombohedra in the crystal structure of $2/1-(Al,Zn)_{3+g}Mg_{2-g}$.



Stability of Fullerenes

2 conformers of C_{240}

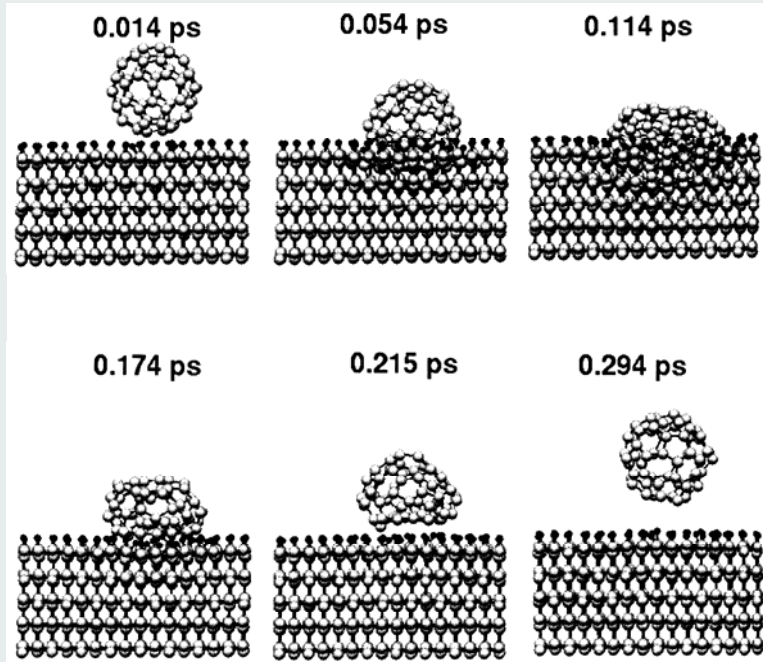
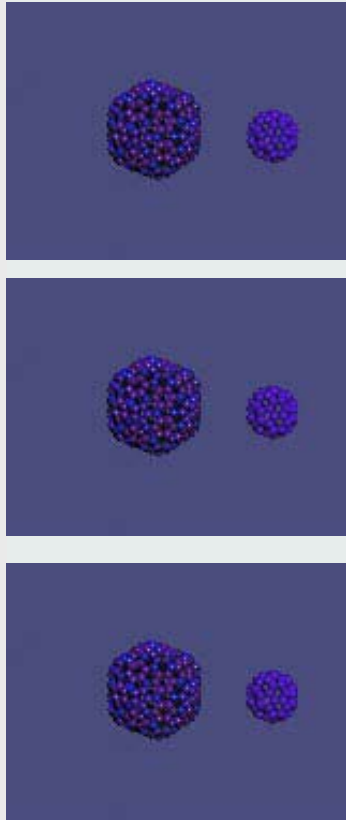


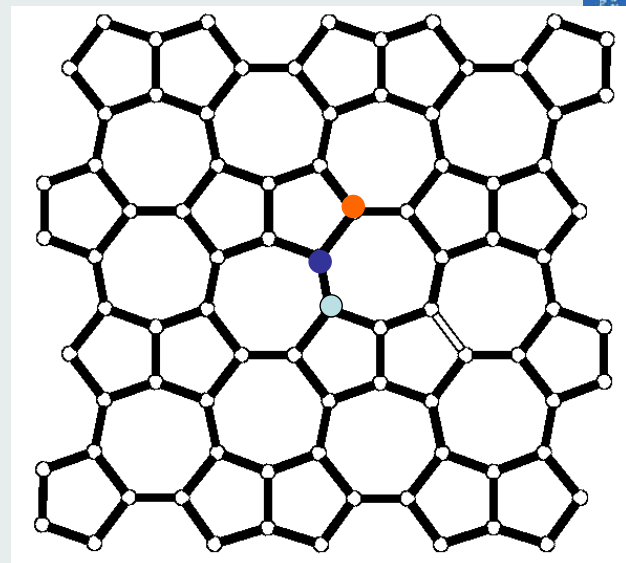
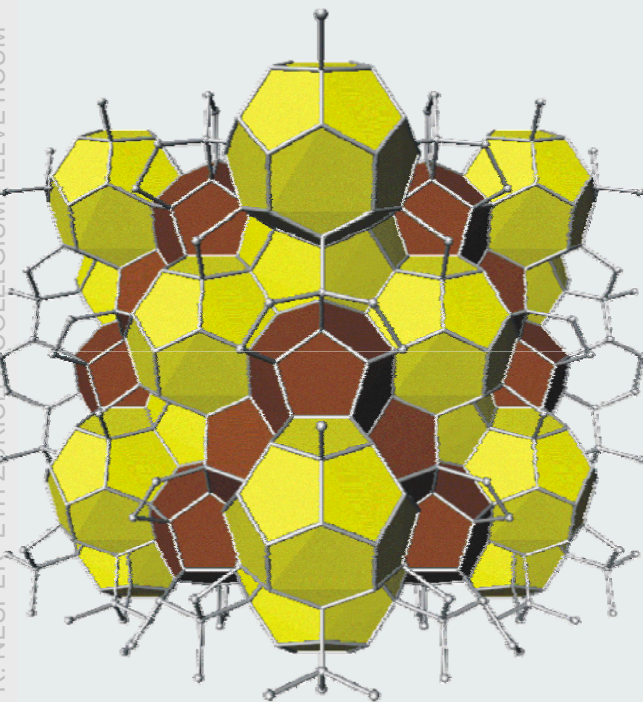
Figure 6.6 Snapshots of a simulated unreactive collision of C_{240} with a hydrogen-terminated (111) diamond surface. The initial collision energy is 250 eV.

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More New Carbons to Come?



(7²⁵) (7⁵⁷) (7⁵²) net

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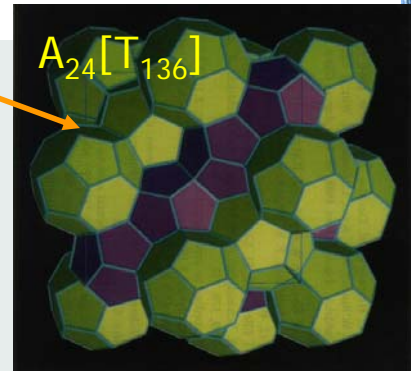
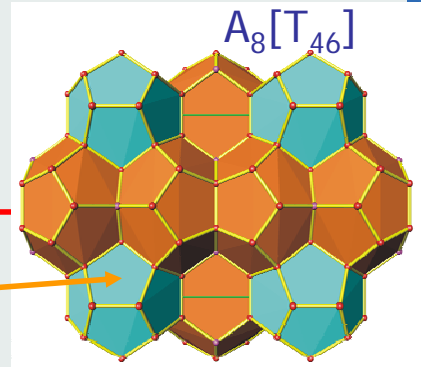
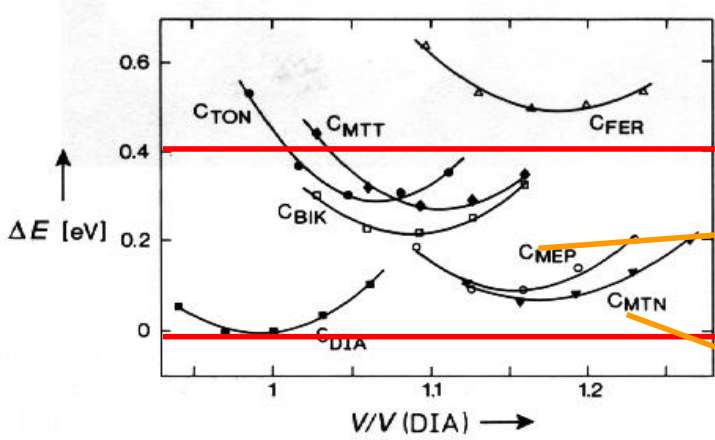
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Hyperbolic 3D Carbons - sp^3 Frameworks

Car-Parrinello-MD based on zeolite trial structures

LVETICUM



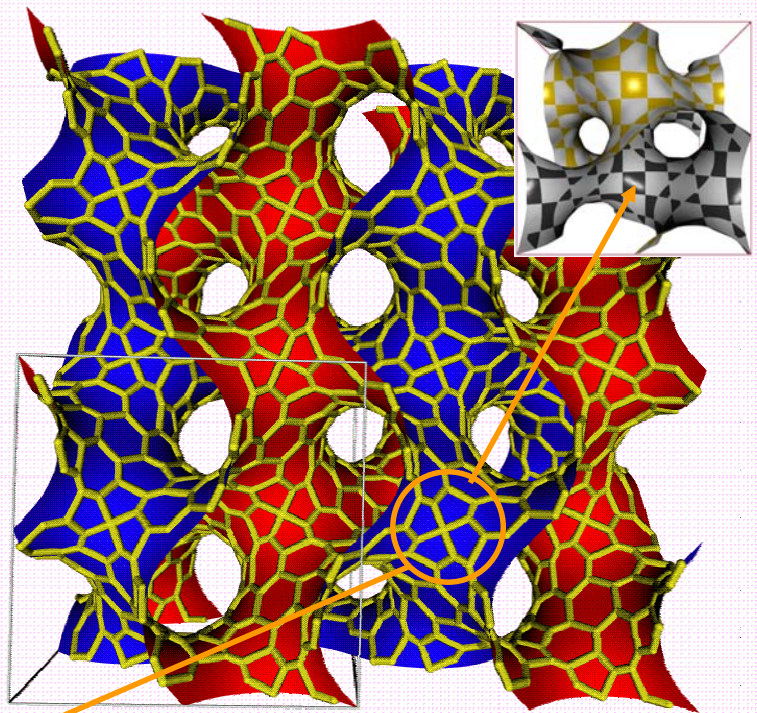
R. Nesper, K. Vogel, P. Blöchl, *Angew. Chem.* 1993, **105**, 786

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Novel Hyperbolic Carbons – sp^2 Frameworks

R. Nesper, S. Leoni
Chemphyschem 2001, **2** (7), 413

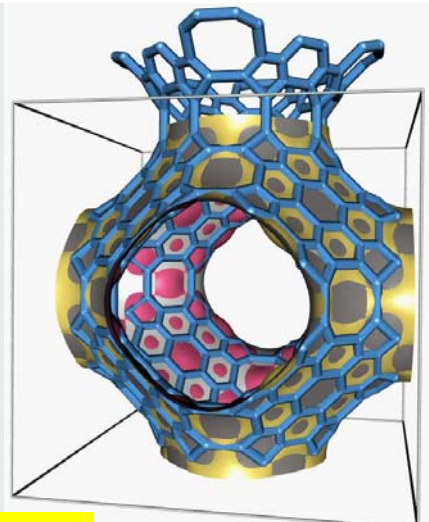
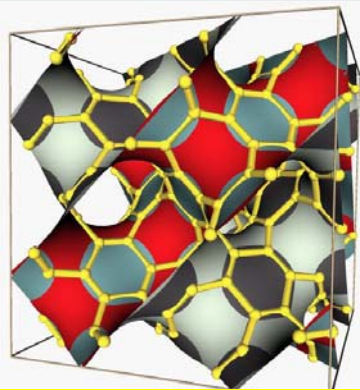
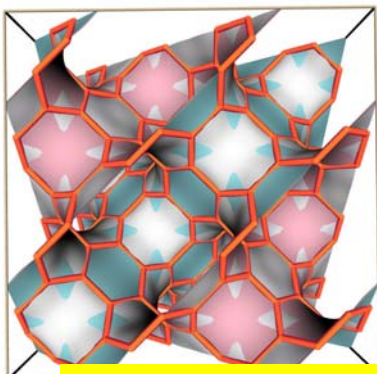


$G[(76^2)(765)(755)(5^4)]$

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More Novel sp^2 Carbons ?



R. Nesper, S. Leoni, *Chemphyschem* 2001, 2 (7), 413

