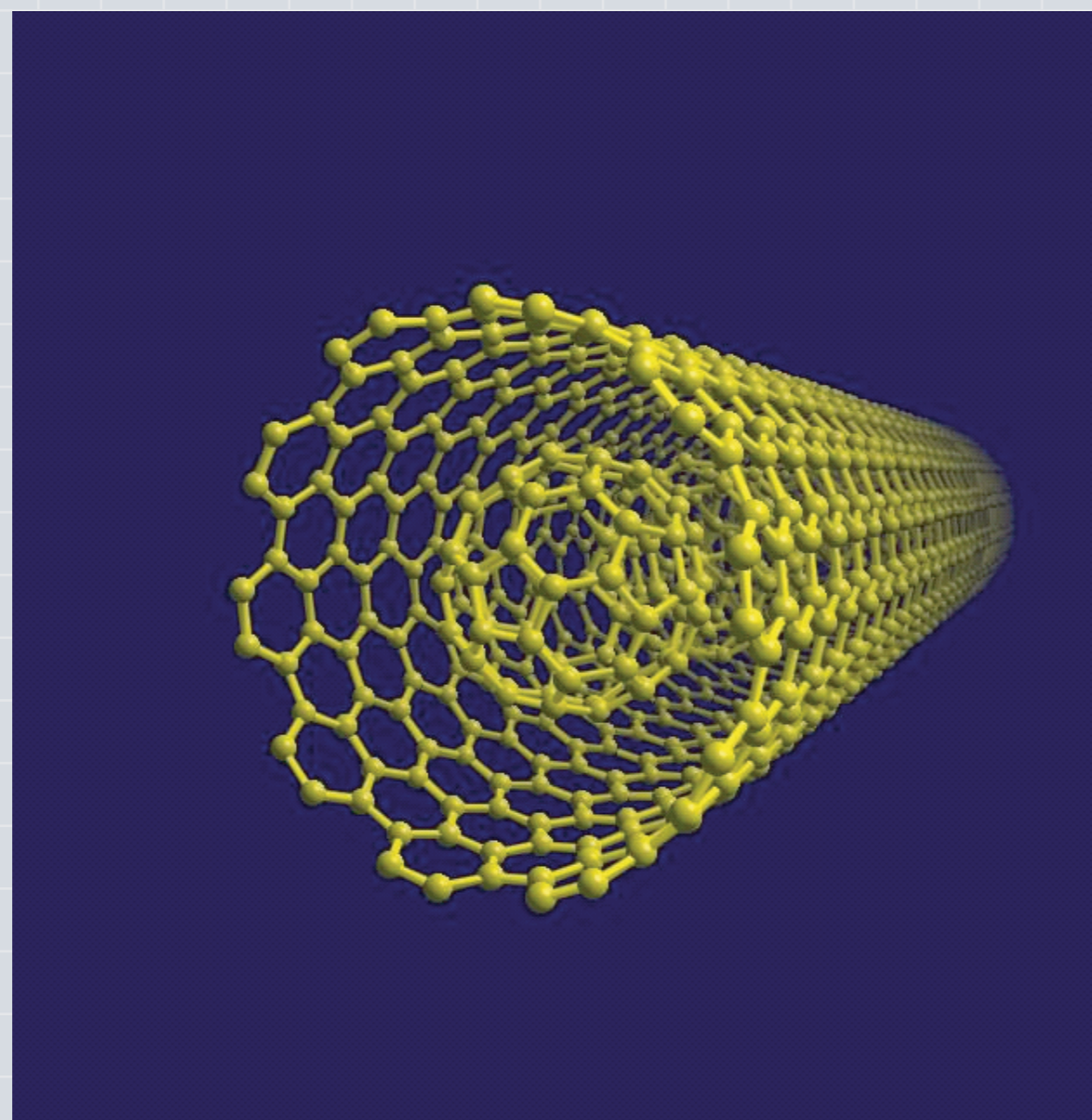


Carbon Nano-Peapods

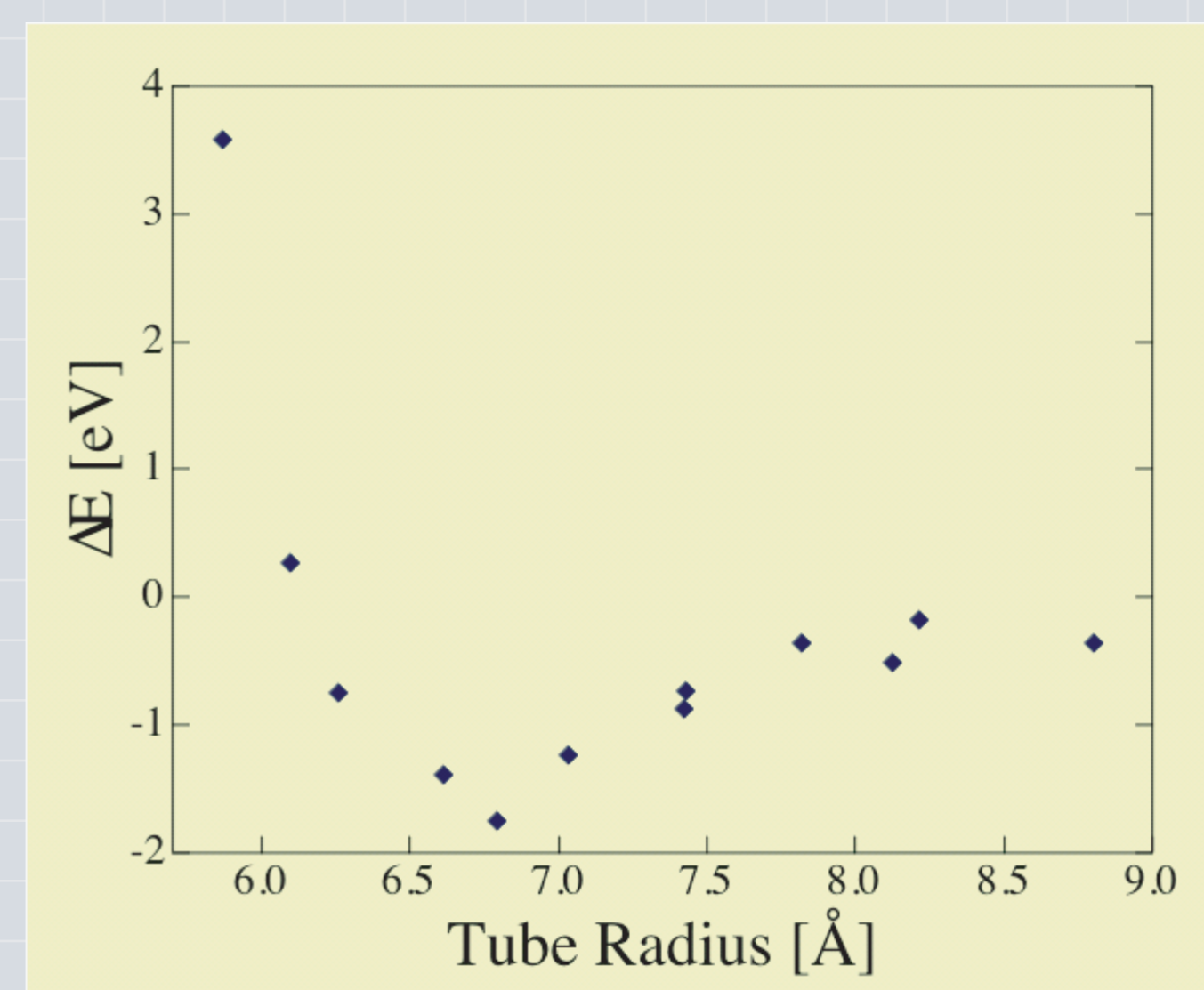
Geometry



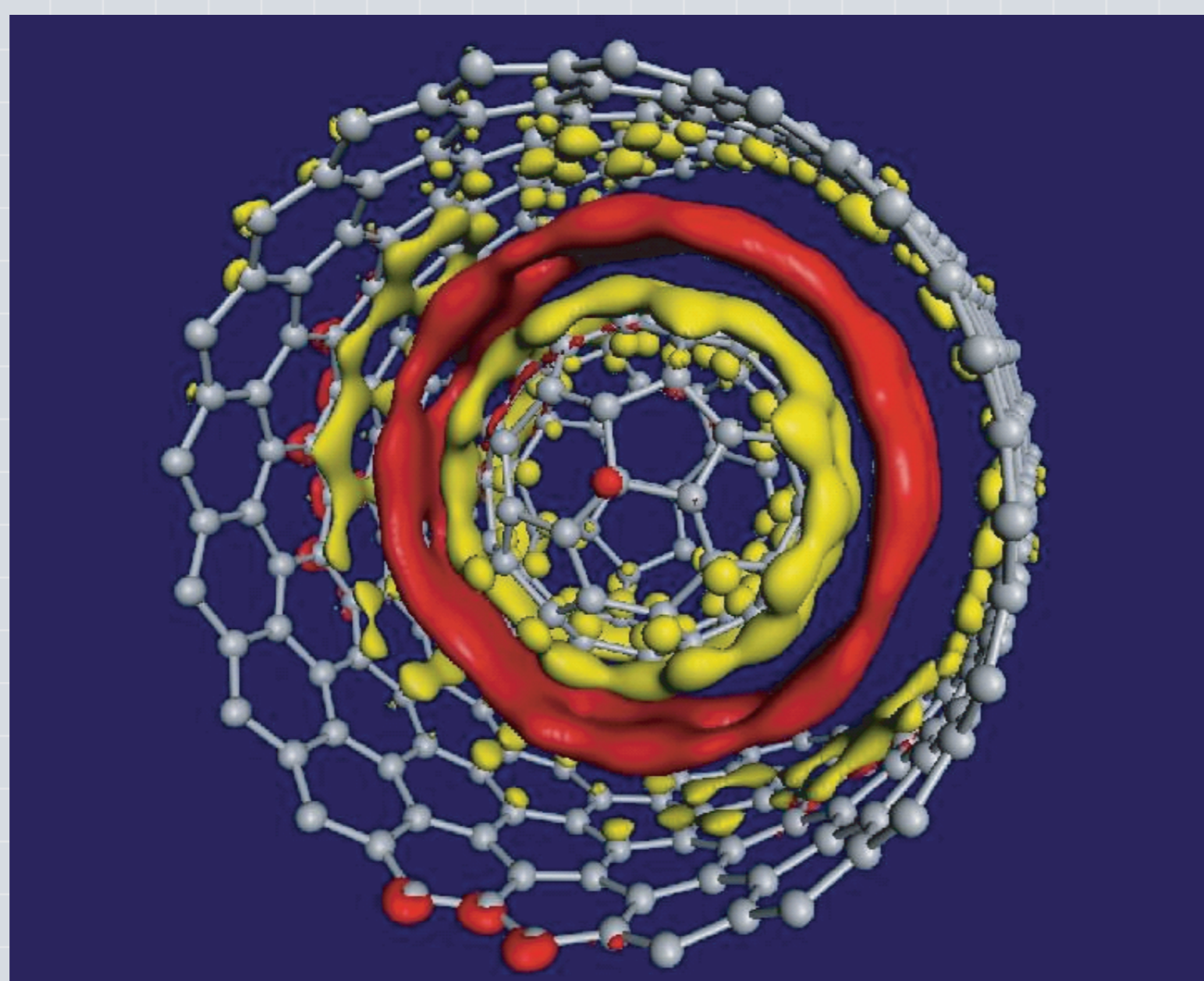
- ▶ **An optimized geometry of a single-walled carbon nanotube containing a row of C₆₀s:** Recently high resolution transmission electron microscope (TEM) images clearly showed the encapsulation of C₆₀s in carbon nanotubes. The unusual nanometer-scale carbon networks are called "carbon peapods" of which structures are characterized by an interesting combination of one- and zero-dimensional constituent units, i.e. carbon nanotubes and fullerenes. The peapods are thus regarded as new hierarchical solids with mixed dimensionality.

Energetics

- ▶ **Reaction Energies (ΔE) per C₆₀ in the encapsulation reaction for carbon nanotube:** We perform the first-principles electronic structure calculations to clarify the energetics of the peapods. The reaction is exothermic for the tubes whose radii are thicker than 6.25 Å. The reaction for the tube with radius of 6.76 Å is found to be the most favorable. The results indicate that the inner space of the nanotube with an appropriate radius is a nano-scale container for fullerenes and other molecules.



Electronic Structure



- ▶ **Isosurfaces of the electron rich area (red) and those of the electron poor area (yellow) than a simple sum of two-self consistent charge densities of the nanotubes and C₆₀:** The charge redistribution shows a role of space between the nanotube and C₆₀. It is clear that the electrons are transferred mainly from the π orbitals of both the nanotube and C₆₀ to the spacious region between the nanotube and C₆₀.