

Topology and Electronic Structure of Nanotube Junctions of Tetrapod Shape

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We propose a series of carbon nanostructure in the shape of tetrapod as a junction for carbon nanotubes. The tetrapod junctions are open networks made of sp^2 carbon atoms, have a negative Gaussian curvature, and connect four nanotubes. We define, in the present study, the standard tetrapod junctions to have twelve heptagons only other than hexagons and to have T_d symmetry. The structure of the standard tetrapod junctions can then be categorized by specifying two topological factors, i.e., the kind of nanotubes and the center of the triangular faces of the skeleton tetrahedron. One can vary the size of the tetrapod junction by specifying another two factors, i.e., the nanotube radius and the size of the triangular faces. The tetrapod junctions form 3D crystal lattices of diamond type which are specified by the length of the nanotubes.

Our tight-binding energy-band calculations for the standard tetrapod junctions of smaller sizes found that the electronic property of the tetrapod junctions mainly depends on the center of the triangular faces: The junctions having a carbon atom in the center of the faces exhibit metallic band structure while the ones having a benzene ring in the center of the faces are semiconductors. We also found that tetrapod junctions connecting (6,0) nanotubes exhibit a flat band near the Fermi energy in a particular region of the momentum space. The origin of the flat band can be figured out from the wavefunction distribution. We also mention the possibility of non-standard tetrapod junctions to connect nanotubes of different kinds and/or different radii.

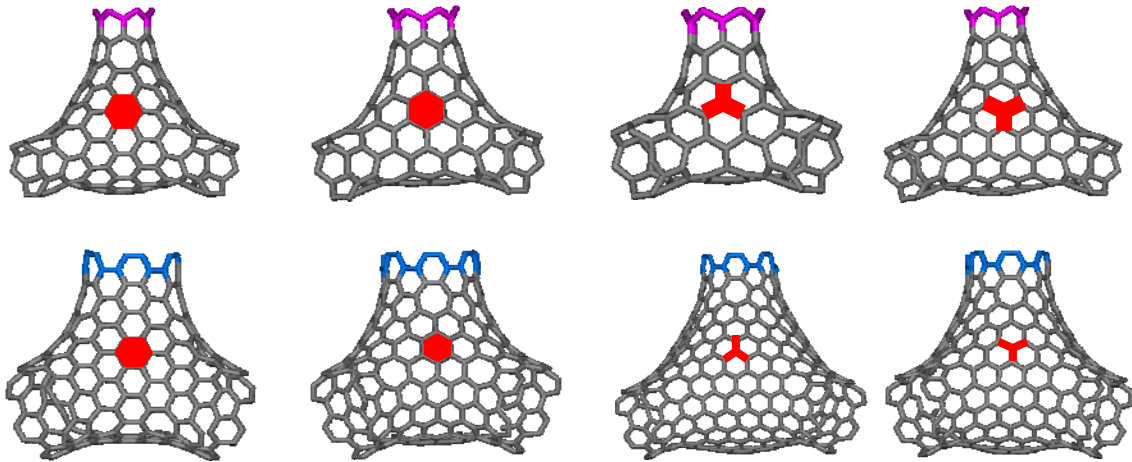


Fig. The standard tetrapod junctions in eight categories.