New carbon forms of polymerized fullerenes or/and single-walled nanotubes (SWNT’s) are considered. Such structures can be produced as a result of different cycloaddition reactions: (2+2), (2+4), (3+3), (4+4) and their combinations.

Computer modeling of geometrical and electronic structures of the following polymer forms are reported:

a) semiconducting solids — close-packed two- and three-dimensional structures based on \((D_{6h})-C_{60}\) (with 12 \(sp^3\) atoms per \(C_{60}\) in 2D phase and with 24 \(sp^3\), and 12 \(sp^2\) atoms per \(C_{60}\) in 3D phase) [1];

b) new semiconducting three-dimensional 3D polymer on the base of \(C_{60}\) formed as a result of several cycloaddition reactions [2];

c) chain and 3D semiconducting structures describing high-pressure and high-temperature \(C_{60}\) phases, and \(C_{3n}\) transformation into \((5,5)\) nanotubes;

d) semiconducting polymer structures on the base of SWNT including structures of \((n,0)\) and \((n,n)\) nanotubes [3, 4];

e) crossing polymerized nanotubes [4].

Some of considered polymer structures have good agreement with experiments of A. Zettl (\(C_{60}\) [5]), \(V.\) Blank (\(C_{60}\) [6] and \(C_{3n}\) [7] materials), and M. Popov (SWNT polymers [8]) groups.

This work was supported by INTAS (00-237), RFBR and RSTP “Fullerene and Atomic Clusters”.


