Chapter 12
Conclusions and Further Outlook

As it has been shown above, a grand variety of carbon allotropes and forms is currently known. They can be very common (graphite, coal) or rare (nanobuds, nanoplates, or nanocups) and can be well-developed industrially (carbon black) or intensively studied on nano-level (carbon nanotubes or graphene), doped with metals and functionalized with organic and organometallic moieties. The hexagonal network of nanotube cylinders, graphene sheets, or fullerene molecules consisting of hexagons and pentagons of carbon atoms are highly aesthetically pleasing, providing inspiration both to artists and scientists [1]. The shape of carbon nanotubes also influences their outstanding physical properties, such as electrical and heat conductance, which are already exceeding many traditional materials, as well as mechanical strength. Fully carbon electronic devices are now a main dream and great expectative of modern technologies, where a lot of researchers are working.

Despite low number of reports, carbon "less-common nanostructures" tend to have much more applications in future. For example, the combination of relatively chemically inert carbon nanotubes and more active fullerenes (carbon nanobuds, CNBs) can be compatible with a variety of other materials, in particular polymers forming composites with enhanced flexibility and sensor characteristics. Among other possible applications, the uncontaminated magnetic nanobuds hold good promise in the field of spintronics. Greater opened space between SWCNTs allows CNBs to be more effective for gas storage.

Coordination and organometallic chemistry of carbon allotropes, in particular graphene and carbon nanotubes, is very important for the following reasons. Metal nanoparticles, atoms, clusters, or cations, being bound with carbon nanostructures directly through M-C σ- or π-bonds or via a ligand group, electrostatic or van der Waals interactions, or charge transfer, are responsible for new properties of formed metal–carbon composites, which are absent in primary carbons. Metals can provide optical, redox, and magnetic activities to the carbon nanostructures. These new properties lead to novel applications, for example, magnetic and photoluminescent properties of endohedral metal fullerenes, novel electrochemical properties of metal-modified glassy carbon, catalytic properties of metal surface-decorated CNT composites, nanoreactor properties of metal clusters embedded within nanotube channel, etc. The chemistry of carbon nanostructures is still limited by many practical peculiarities, such as lack of purity, polydispersity, or structural complexity. New horizons for these fascinating carbon materials can be open upon more profound understanding of bonding and interactions M-C in these composites. Any application of metal complexes could be extrapolated to their carbon-containing composites, since these materials have and could have a host of applications in many fields, such as drug delivery [2], devices, sensors, catalysis on supporting materials (due to the presence of metallic ions and carbon support), and water treatment (using porous carbon structures), among others.

Applying modern computational methods, a host of new carbon nanoforms (e.g., novamene [3] or protomene [4]) are possible, which have not yet been observed experimentally. In this respect, an efficient and reliable methodology for crystal structure prediction was developed [5], merging ab initio total-energy calculations and a specifically devised evolutionary algorithm. This method allows one to predict the most stable crystal structure and a number of low-energy metastable structures for a given compound at any *P-T* conditions without requiring any experimental input. While in many cases it is possible to solve crystal structure from experimental data, theoretical structure prediction is crucially important for several reasons.

The area of carbon allotropes is currently one of most dynamically developing fields of science and technology, leading to new horizons of the progress. It could be proposed that such trends will remain in the next 10–20 years.

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