Molecular dynamics simulation of carbon nanostructures

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Molecular dynamics calculations can reveal the physical and chemical properties of various carbon nanostructures or can help to devise the possible formation pathways.

In our days the most well known carbon nanostructures are the fullerenes and the nanotubes. They can be thought of as being formed from graphene sheets, i.e. single layers of carbon atoms arranged in a honeycomb lattice. Usually the nature does not follow the mathematical constructions. An ideal nanotube can be thought of as a hexagonal network of carbon atoms that has been rolled up to make a cylinder. There is not any theory of carbon nanotube formation which is based on this construction. Although the first time the C60 and C70 were constructed by laser irradiated graphite, the fullerene formation theories are based on various fragments of carbon chains, and networks of pentagonal and hexagonal rings.

In the present talk various formation pathways for carbon nanostructure formations will be studied in the frame work of molecular dynamics calculations. Suggestions will be given for practical experimental realizations.