Molecular Dynamics Simulations of Picotube Peapods

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Motivation
Carbon picotubes are a promising starting point for the specific synthesis of nanotubes. One potentially useful configuration evolves from inserting picotubes into a nanotube. In this context the interaction between nanotubes and picotubes is of particular interest.

Simulations
We place three Tetramer picotubes in a (9,9) nanotube. Temperatures between 100 K and 3000 K are simulated. All calculations are performed with the molecular dynamics package pdynamo, using the semiempirical quantum chemical model AM1 for the energy calculations. Structural studies of picotubes show an excellent agreement between our results and DFT calculations.

Initial configuration of the Tetramer picotubes in the nanotube. The type of nanotube is chosen such that the distance between the nanotube wall and the hydrogen atoms at the wings of the tetramer slightly exceeds the carbon-hydrogen-bondlength.

We observe three effects

Oscillations of the picotubes inside the nanotube at up to 600 K

A directional transport of the picotube molecules starting at 800 K

A structural reorganisation of the picotubes towards short nanotubes above 2000 K

Top and side view of a Tetramer picotube as calculated with the pdynamo code. This fully conjugated hydrocarbon which strongly resembles a short (4,4) nanotube has been successfully synthesized in 1996.

When heated to 600 K the molecules perform an inversely phased rotation.

At 2500 K the open picotube transforms to a closed configuration, e.g. a very short (4,4) nanotube.

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Our studies clearly show a directional movement of the picotube molecules through the nanotube. The velocity increases in a range of 1000 - 2000 m/s with increasing temperature.

All picotube molecules move in phase.

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References

Outlook
Find suitable conditions for the synthesis of a long inner nanotube.
Study the conditions for the transport of picotubes through the nanotube.