

Systematic Enumeration of Carbon Nanothreads

Scientific Achievement

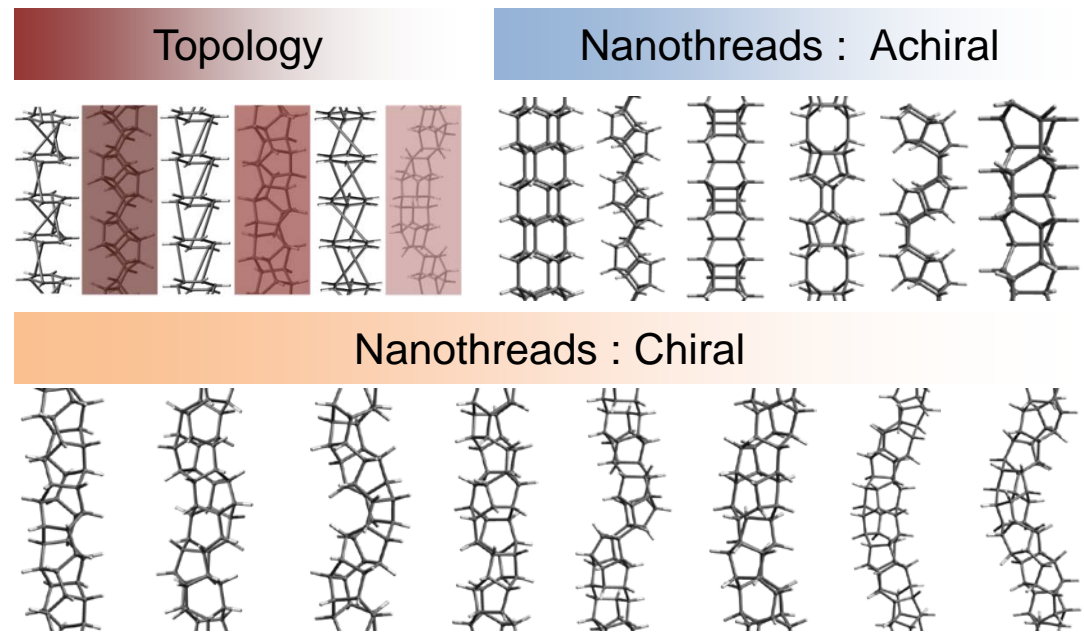
Enumeration of candidate atomic structures of carbon nanothreads, especially low energy structures.

Significance and Impact

This theory study will aid in the experimental determination of nanothread structure, guide modeling of properties, and inspire new directions in nanothread synthesis beyond those employing benzene precursor.

Research Details

- 15 nanothreads close in energy to the most stable one were identified.
- Materials properties such as bandgaps and mechanical stiffness were modeled; some nanothreads were found to be as strong as sp^2 carbon nanotubes.
- Euler's rules for ring counting were generalized to guide structure design of nanothreads synthesized from molecules other than benzene.



Xu, E.-S., Lammert, P.E. and Crespi, V.H. Systematic Enumeration of sp^3 Nanothreads. Nano Letters, 10.1021/acs.nanolett.5b01343(2015).



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