

Mechanisms for Nanothread Formation

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Scientific Achievement

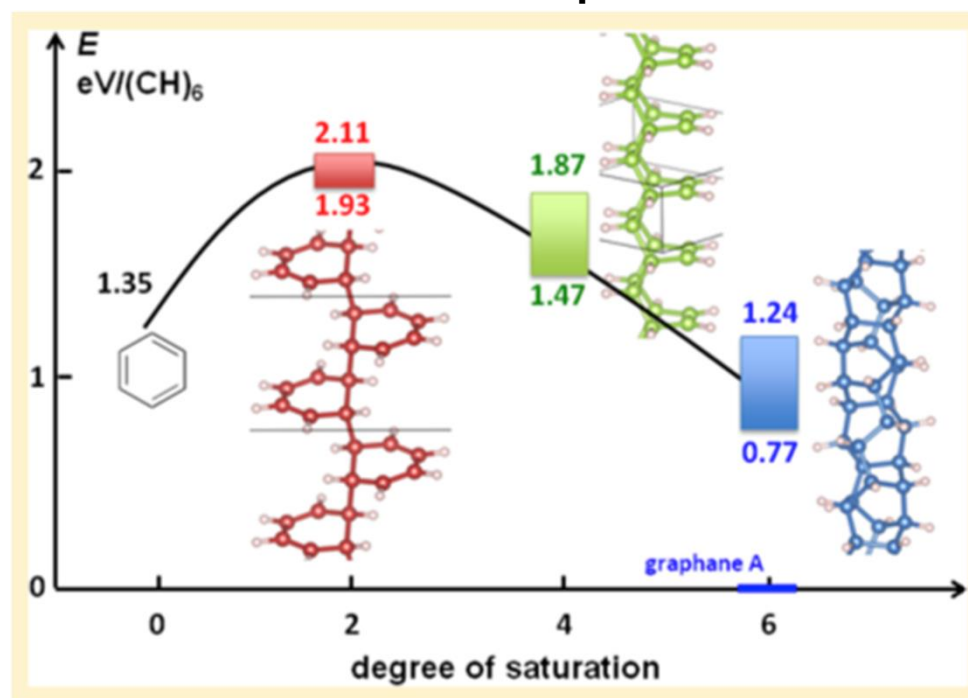
Elucidation of plausible reaction mechanisms that convert benzene molecules into saturated sp^3 carbon nanothreads.

Significance and Impact

Understanding the kinetic barriers to the formation of carbon nanothreads is an important step in narrowing the set of possible structures from those that are possible to those that are probable.

Research Details

- “ Identification of Degree-2 and Degree-4 intermediates to stepwise saturation of benzene molecules.
- “ Propagation of partially saturated polymers and cycloaddition reactions can lead to nanothread formation.
- “ Database of structures allows comparison of energies between intermediate structures and other $(CH)_n$ species.
- “ Plane-wave pseudopotential method for accurate evaluation of total energies of intermediate polymers and saturated nanothreads .



Chen, B.; Hoffmann, R.; Ashcroft, N.W.; Badding, J.V.; Xu, E.; Crespi, V.H. Linearly Polymerized Benzene Arrays as Intermediates, Tracing Pathways to Carbon Nanothreads. *J. Am. Chem. Soc.* 137,14373-14386 (2015). DOI: 10.1021/jacs.5b09053.