

## How does hydrogenation change carbon nanotubes?

### NSF-NSEC: Center for High-rate Nanomanufacturing

**Objective:** Develop a method and provide fundamental understanding of the way to separate carbon nanotubes from a bundle by covering it with atomic hydrogen by a wet chemical process in a solution.

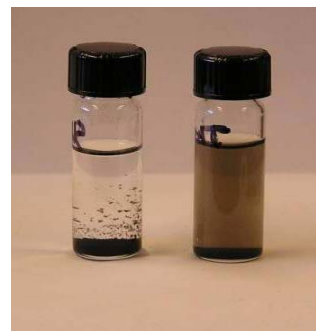
**Broader Impact:** Developing a new way to separate carbon nanotubes from bundles addressed a major problem in nanotechnology using nanotubes

### Significant Results:

- Separation of nanotubes in bundles upon exposure to high boiling polyamines as hydrogenation reagents has been demonstrated.

*Figure:*

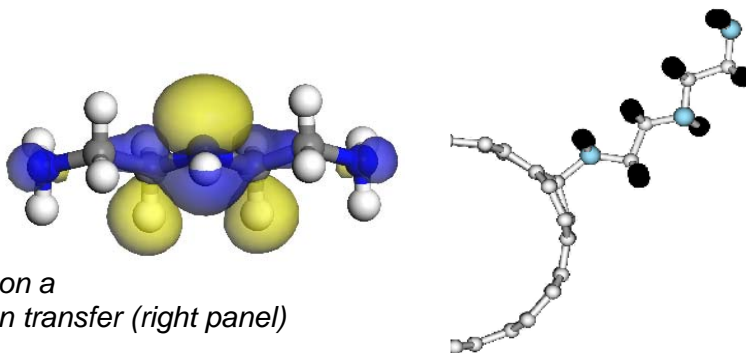
*Untreated nanotubes in the left vial form heavy bundles and sink to the bottom. Hydrogenated nanotubes in the right vial remain suspended several days after treatment*



- The fundamental process of transferring hydrogen atoms from polyamines to the contacting nanotube has been understood theoretically

*Figure:*

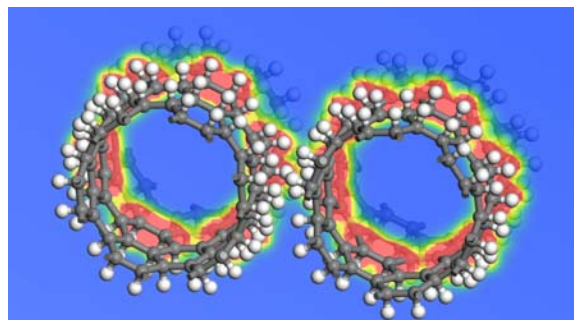
*Equilibrium atomic structure superimposed with the distribution of electrons in the highest occupied molecular orbital of the diethylenetriamine molecule (left panel). Likely docking geometry of this molecule on a carbon nanotube, causing hydrogen transfer (right panel)*



- Calculations suggest that carbon nanotubes should deform when covered by hydrogen

*Figure:*

*Equilibrium structure and electron distribution on nanotubes covered by hydrogen atoms (white spheres)*



[Glen P. Miller, Jeremy Kintigh, Eunja Kim, Philippe F. Weck, Savas Berber, and David Tománek, Hydrogenation of Single-Wall Carbon Nanotubes Using Polyamine Reagents: Combined Experimental and Theoretical Study, J. Am. Chem. Soc. \*\*130\*\*, 2296 \(2008\).](#)