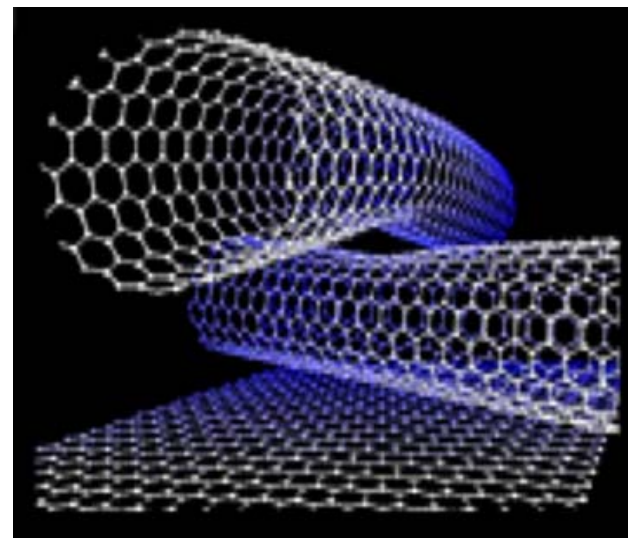


# Functionalization of Carbon Nanotubes via the Diels-Alder Reaction

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**JIN Fellow**  
**Chemistry**  
**May 31, 2005**

- Discovered in 1991  
(Iijima, S.; Ichihashi, T. *Nature* **1993**, 363, 603)
- Unique structure
- Extraordinary properties
- Wide variety of applications
- Insoluble in all media
- Functionalization often destroys desirable properties

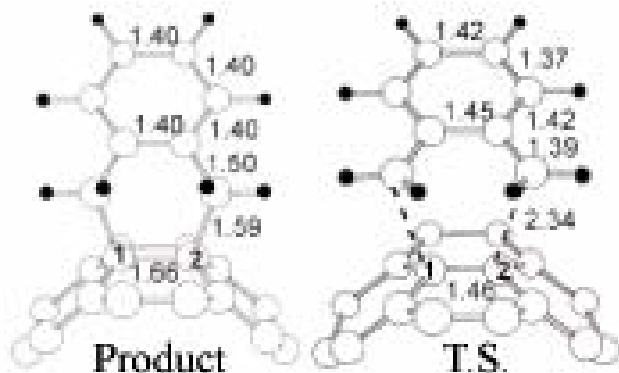


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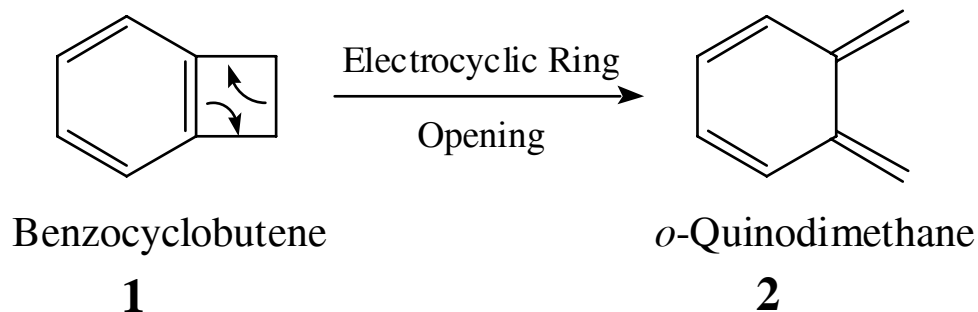
# Functionalization of Carbon Nanotubes via the Diels-Alder Reaction

Zhang, Q. *et al. Org. Lett.* **2002**, 4, 4313



		1,3 butadiene	quinodimethane
SWNT (5,5)	$E_a$ (kcal/mol)	32.4	17.9
	$E_r$ (kcal/mol)	-1.6	-30.1
Ethylene	$E_a$ (kcal/mol)	22.4	8.5
	$E_r$ (kcal/mol)	-43.1	-70.9

ONIOM (B3LYP/6-31G\*:AM1) treatment 130-C fragment metallic (5,5) armchair CNT



Potential Benefits:

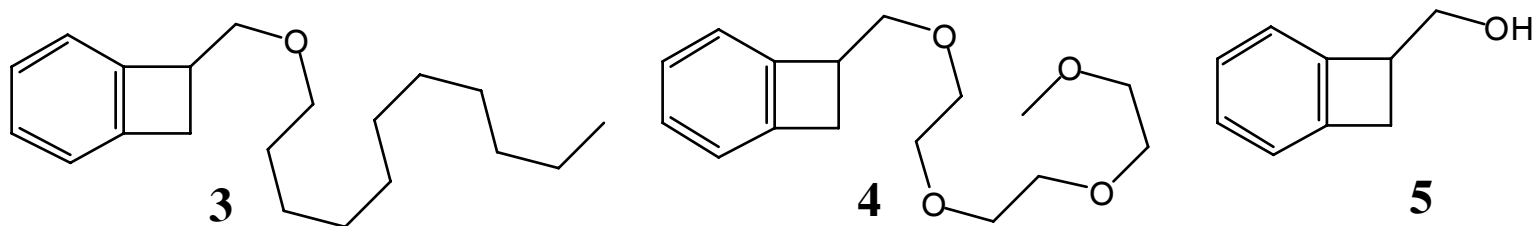
- Low surface coverage
- Variety functional groups
- Crosslinking
- Reversibility



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# Functionalization of Carbon Nanotubes via the Diels-Alder Reaction



## Test Reactions:

- BCB:  $10^{-2}$  -  $10^{-4}$  M **3**, **4**, or **5** in 1,2-dichlorobenzene
- 5-10 mg SWCNT
- Reflux 72 hr, or 1 hr Focused Microwave Reactor
- Filter to obtain CNT mats
- No soluble CNTs

## Future Work:

- Degree of functionalization
  - FT-IR
  - Raman
  - Scanning probe microscopy
- Trapping studies
- In situ spectroscopy

## Acknowledgements:

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- CNT

