



Designing nanowires with tunable semiconducting properties

Objective:

- Design semiconducting nanowires as interconnects in a new generation of nanoelectronics
- Assist NSEC co-PI Glen Miller in synthesizing nanowires with specific semiconducting properties

Approach:

- *Ab initio* quantum chemical calculations yield equilibrium atomic positions and determine if nanowires are metallic or semiconducting

Significant Results:

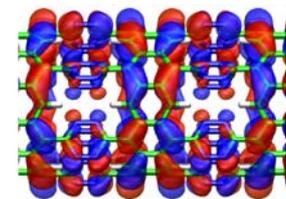
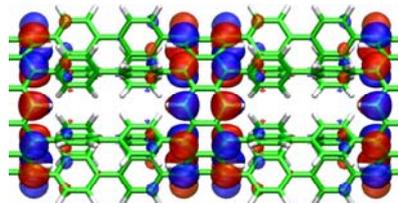
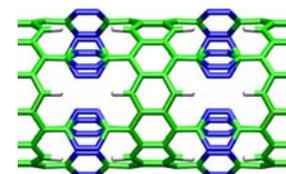
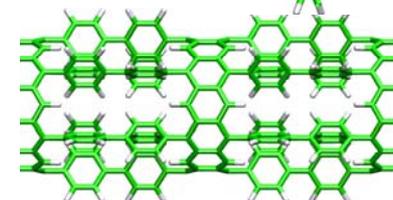
- Suitable candidate nanowires have been identified, consisting of cyclacene molecules connected by linker molecules
- Tunable semiconducting properties can be achieved by using tetrazine molecules as linkers
- *Glen P. Miller, Shinya Okano, and David Tománek, Toward uniform nanotubular compounds: Synthetic approach and ab initio calculations, J. Chem. Phys. 124 121102 (2006).*

Nanowires containing:

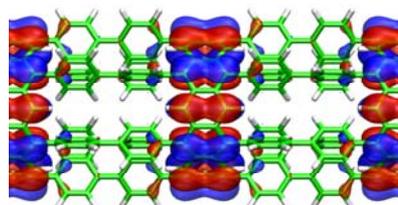
biphenyl linkers:



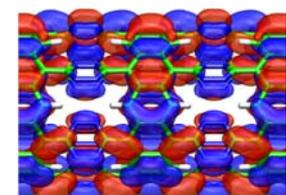
tetrazine linkers:



Charge distribution in quantum states responsible for conduction



Not suitable as nanowire



Suitable nanowire with tunable properties