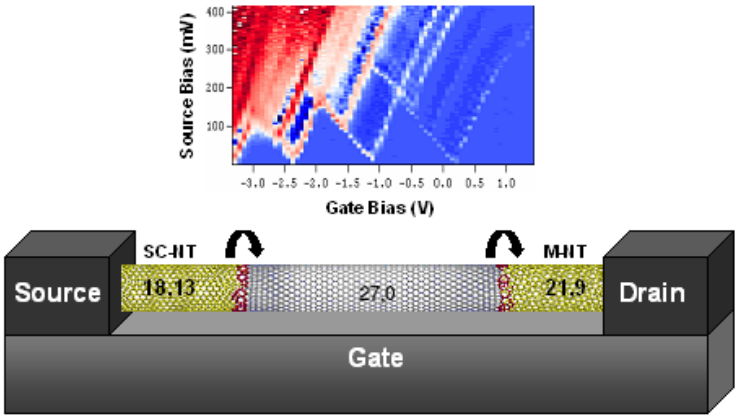
Experimental and theoretical studies of molecular-scale quantum dots at carbon nanotube heterojunctions

Bhupesh Chandra[1], Joydeep Bhattacharjee[2], Young-Woo Son[2], Jeffrey. B. Neaton[2], James Hone[1]
[1]Columbia University, Department of Mechanical Engineering and NSEC
[2]Molecular Foundry, Lawrence Berkeley National Laboratory

Carbon nanotubes can be either semiconducting or metallic depending on their specific crystal structure, or chirality, and thus hold promise for electronics applications because most elements of integrated circuitry can be constructed from CNTs alone.

A related, but distinct and largely unexplored class of nanostructures are carbon nanotube heterojunctions- robust covalent nanoscale interfaces connecting tubes of different chiralities. There have been very few studies of these systems in the literature, and their structural and electronic properties still remain poorly understood, mainly because of their rare occurrences and the challenges associated with their synthesis, characterization and electrical measurements. In particular, there has been only one reported measurement of electrical transport in such a structure, and no study has (until now) provided independent confirmation of a chirality change. In addition to their clear relevance to nanoelectronics, these nanoscale covalent heterojunction interfaces also provide ideal test beds for fundamental studies of molecular-scale transport.

We used a combination of experimental measurements, atomistic modeling, and electronic structure calculations to study a well-characterized nanotube heterojunction. The chiralities of the nanotubes were indexed with Rayleigh scattering and confirmed by the transport measurements on both metal and semiconducting sides, making our device one of the most well characterized composite nanostructures that has ever been studied. Most interestingly, transport measurements through the heterojunction reveal for the first time an all-carbon molecular-scale quantum dot arising exclusively due to the arrangement of defects required to form the heterojunction interface. A detailed atomistic theory that complements our experimental measurements provides a general framework underlining guiding principles to make molecular-scale quantum dot devices from carbon nanotube heterojunctions.



Chandra, B., et al., *Molecular-Scale Quantum Dots from Carbon Nanotube Heterojunctions.* Nano Letters, 2009. **9**(4): p. 1544-1548.