

Molecular Wires: From Self-Organization to Functional Nanosystems

Nanometer-scale materials can have unique properties due to their reduced dimensions, and could serve as building block for the assembly of miniature functional systems. In macroscopic functional systems, wires, tubes and rods play critical roles of transporting energy, forces, matter and information. Which materials could play analogous roles at the smallest possible scale? How does the reduced dimensionality determine the properties of molecular wires? How can they be organized and integrated into functional systems?

My research focuses on the organization of molecular wires and one-dimensional nanostructures, such as carbon nanotubes, inorganic nanowires and polymers, their integration into functional nanosystems¹ (mechanical, electronic, electromechanical, optoelectronic, electromagnetic, thermal, etc.), and their characterization by mechanical and electrical measurements at the nanometer scale.

One of our innovations has been the development of epitaxial approaches to carbon nanotube organization, namely, the directed growth of carbon nanotubes by well-defined crystal surfaces. Starting with the first observation of catalytic nanotube growth along atomic steps², we subsequently identified three different modes of orientational ‘nanotube epitaxy’: ‘Lattice-directed nanotube epitaxy’ (by atomic rows), ‘ledge-directed nanotube epitaxy’ (by atomic steps)²⁻⁴ and ‘nanotube graphoepitaxy’ (by nanofacets)⁵. In addition, we combined these modes of nanotube epitaxy with two types of external aligning forces: electric field⁶ and gas flow. This enabled the controlled formation of a variety of previously unattainable morphologies of nanotubes arrays⁷, including highly straight, kinked, wavy, crossed⁸, serpentine⁹ and looped.

A second contribution has been the first study of the effect of torsion on the electronic properties of carbon nanotubes, which led to the observation of torsional electromechanical quantum oscillations in carbon nanotubes¹⁰. We found that continuously varying the chirality of a nanotube by mechanical torsion¹¹ can induce conductance oscillations, which can be attributed to metal-semiconductor periodic transitions. The phenomenon is observed in multi-walled carbon nanotubes, where both the torque and the current are shown to be carried predominantly by the outermost nanotube wall. The oscillation period with torsion, and its dependence on the nanotube diameter¹², is consistent with the theoretical shifting of the corners of the first Brillouin zone of graphene across different subbands allowed in the nanotube. Beyond a critical torsion, the conductance irreversibly drops due to torsional failure, allowing us to determine for the first time the torsional strength of carbon nanotubes. Our results suggest that carbon nanotubes could be used as self-sensing torsional springs for nanoelectromechanical systems. Recently, we have extended our torsional mechanical studies to inorganic nanotubes¹³.

A third contribution was generalization of the nanotube epitaxy idea to other types of molecular and nanoscopic one-dimensional structures. Spontaneously restructured crystal surfaces serve as self-assembled templates for the generation of unprecedentedly dense stripe-patterned self-assembled monolayers, as well as parallel and crossbar periodic arrays of gold nanowires and nanogrids, as well as silicon nanotrenches and nanowaffles^{14,15}.

Other contributions include studies of single-polymer dynamics and their application to molecular recognition imaging¹⁶, and theoretical studies relating the chemical reactivity of carbon nanotubes to their electronic structure^{17,18}.

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