Bottom Up Assembly of Metal and Semiconductor Nanowires: Fundamental Forces to Nanoelectronic Circuits

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PIs: **Darrell Velegol, Kristen A. Fichthorn, Theresa Mayer, Christine D. Keating**
The Pennsylvania State University, University Park PA 16802

Goal: Bottom-up assembly of a nanoscale logic circuit

Miniaturization of computer and consumer electronics faces a huge hurdle: making circuits with critical dimensions less than ~150 nm. Not only would such "nanocircuits" increase chip density, but they could exploit important quantum phenomena not possible with current devices. While well-known techniques (e.g., photolithography) are used to produce transistors and computer chips, newer techniques (e.g., DNA-directed assembly of nanospheres[1], carbon nanotubes) have been used to create simple lab-scale nanodevices. Top down techniques for creating nanodevices (e.g., atomic force microscopy, e-beam lithography) are slow and expensive, making them infeasible for bulk production. And so three key barriers remain for nanocircuit fabrication: 1) miniaturization below 150 nm sizes, 2) increased circuit complexity and intra-device chemical specificity, and 3) going from lab scale to production scale.

We are developing the bottom up, DNA-directed assembly[2] of "designer nanowires" to produce a nanoscale logic circuit. The nanowires can be 20 to 500 nm in diameter and almost any length, with even individual wires having multiple materials (e.g., platinum, gold, semiconductors). The wires will be assembled in any configuration – with chemical specificity – using DNA as a "selective glue".

Bottleneck to mass production of functional assemblies: control of fundamental forces.

Bottom-up assembly requires both enhancement of the forces directing the assembly process, as well as the reduction of nonspecific physical forces that cause the premature (and undesired) aggregation of the particles. The generation of *functional* assemblies for nanoscale electronic devices further requires appropriate building blocks, such as the nanowires described in this proposal. For these particles, the interplay between desired selective assembly forces (e.g., DNA as a "selective glue") and undesired nonspecific aggregation (e.g., van der Waals forces) is particularly challenging. This is due to the large contact areas (as compared to spheres), high mass, and large Hamaker constants associated with metallic nanowires. We will address these challenges with a combined experimental and modeling approach designed to produce significant improvements not only in directed assembly, but also in our understanding of the process and our ability to predict optimal conditions for future assembly targets.

Approach: Enable bottom-up assembly by engineering fundamental forces nanocolloids forces – van der Waals, solvation, depletion, DNA binding.

The key to this proposal is to develop bottom-up DNA-directed assembly of the various types of nanowires, while preventing undesirable aggregation due to nonspecific forces. This proposal has five objectives, each requiring various expertise, which will be studied in parallel:

1. ***Build a simple nanoelectronic logic gate based on Binary Decisions Diagrams (BDD) using electric field-induced nanowire alignment, to develop integration and characterization procedures.***

2. ***Assemble a similar BDD circuit using bottom-up techniques at the nanoscale, by enhancing nondeterministic "bead templating" with phase diagrams from measurements and modeling.***
3. ***Obtain predictive models for nanoparticle forces by synergizing measurements and modeling, enabling the logical choice of co-solvents, T, particles, etc. in a huge parameter space.***
4. ***Engineer the technique of DNA-directed assembly to build bulk quantities of complex nanocircuits.***
5. ***Improve the public's confidence to make ethical and voting decisions about nanotechnology through local "hands-on" workshops and "teaching teachers to teach nano" in k-12 schools.***

Key research results

Velegol's research has focused on two major research activities. First, we have improved our method for measuring interparticle forces using "particle force light scattering" (PFLS). We have measured interparticle forces for sub-micron particles, and we are extending to nanometer-scale particles. Measurements of nanocolloids forces – the first anywhere – will enable us to assess heuristics from the Fichthorn and Keating groups for stable dispersions of various particle-solvent systems. Several companies have recently inquired about stabilizing nanocolloids without dispersants.

Second, the Velegol lab is developing a technique for synthesizing "colloidal molecules", which are colloidal assemblies that have particles bonded at designed angles and distances. Just as a water molecule has an oxygen and two hydrogens attached at an angle of 104.5 degrees, we are now able to do site-specific chemistry with colloidal particles. This is an important advance over previous researchers, who primarily worked with closed-packed particles. The Velegol group has filed a provisional patent on synthesizing colloidal molecules, and this work is already leading to entirely new research projects. Part of the work is being done at the Penn State Nanofabrication Facility.

Fichthorn's research has focused on two areas. The first of these is modeling the assembly of nanoparticle rods and spheres, as well as the templated assembly of nanorods by micron-sized spheres, using Monte Carlo simulations. To date, the Fichthorn group has developed and tested Monte Carlo code for modeling hard-sphere assemblies. In the near future, this code will be used to understand the phase behavior of rod-sphere mixtures as a function of rod aspect ratio, rod length relative to sphere diameter, mole fraction of each object, etc. Such phase diagrams can be compared to experimental studies from the Keating group.

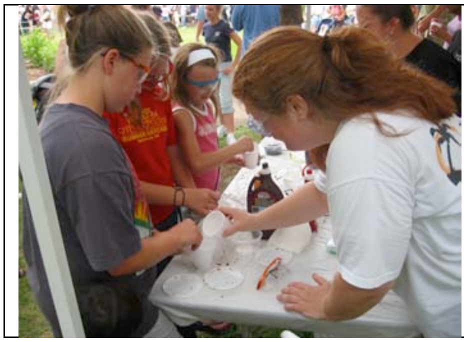
In a second area of emphasis, the Fichthorn group has been using molecular-dynamics simulations to model solvation forces between colloidal nanoparticles. These studies have revealed the influence of nanoparticle size, shape, surface roughness, nanoparticle-solvent interactions, as well as solvent molecular structure on solvation forces and suggest that nanoparticle suspensions can be engineered to achieve selective assembly and dispersion. Results from these calculations will be used in coarse-grained Monte Carlo simulations of nanoparticle dispersions. In addition, the results from these calculations can be compared to experimental results from the Velegol group.

The Mayer group has engaged in research to integrate and characterize silicon nanowire (SiNW)-based field effect transistors, which will be used as a fundamental building block of the bottom up architectures that are being investigated in this program. In collaboration with the Redwing group, SiNWs that are grown by incorporating intentional p- and n-type dopants using trimethylboron and phosphine sources were investigated by fabricating test structures and measuring 4-point resistance and gated conductance of a statistically significant number of nanowires of each doping type and density. It was demonstrated that the SiNWs have a nominal p-type background doping and that the incorporation of phosphorous can be used to convert the SiNWs from p- to n-type. This is a significant result for this project because complementary field effect devices are required for the proposed simple circuit demonstration. As part of this study, we also determined that the nanowire conductance is strongly dependent on the ambient in which the SiNWs are measured. This is a result of the high density of surface states present on the SiNWs. We are currently investigating incorporating hydrogen annealing and dry oxidation of the nanowires to form a high quality passivating oxide that can also serve as a gate dielectric for gate-all-around field effect devices.

In a second area of research, the Mayer group has been collaborating with the Redwing group to develop methods for producing monodisperse suspensions of SiNWs. This involves incorporating a Ge nanowire segment at the base of the SiNW. Ge was selected because it can be etched selectively (>1000/1) relative to Si in warm H2O2. Preliminary results show that the SiNW segments can be removed from the growth substrate using this technique. This control over nanowire length is important for the assembly aspect of this NIRT program.

Key broader impact activities

Several members of our NIRT team (e.g., PhD students Allison Yake, Charles Snyder, Tsung-ta Ho, and Lisa Dillenback) participated in the Central Pennsylvania Festival of the Arts, at a booth worked in synergy with the MRSEC team in Nanoscale Science and Engineering here at Penn State. Typically about 200,000 people attend this event, and this year the estimate is that about 1000 children attended the booth (see Figure).



Children see how to make ice cream by forming crystals with liquid nitrogen. Over 1000 children came by the Nanoscale Science and Engineering booth, in which our NIRT participated. The booth was coordinated primarily by the Penn State MRSEC on Nanoscale Science & Engineering.

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[1] Park, So-Jung; Taton, T. Andrew; Mirkin, Chad A. “Array-Based Electrical Detection of DNA with Nanoparticle Probes.” Science, 295, 1503 (2002).

[2] Nicewarner-Pena, Sheila R.; Freeman, R. Griffith; Reiss, Brian D.; He, Lin; Pena, David J.; Walton, Ian D.; Cromer, Remy; Keating, Christine D.; Natan, Michael J. “Submicrometer Metallic Barcodes.” Science, 294, 137 (2001).