LA-SiGMA

Louisiana Alliance for Simulation-Guided Materials Applications

Aggregation and its Mitigation in Graphene Nanoribbons

– Paulette Clancy, Cornell University

SEMINAR
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APRIL 22
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3:00 PM

One of the chief difficulties of incorporating graphene into logic devices is its intrinsic lack of a band gap. One solution involves the formation of nanoribbons (GNRs). GNRs are commonly created through lithographic techniques or the longitudinal unzipping of carbon nanotubes.

We are using Molecular Dynamics (MD) methods and free energy techniques to address an aggregation issue that is a major limiting factor to our ability to create GNR devices. Specifically, we will be looking at GNRs synthesized by oxidizing soluble precursor poly(o-phenylene) polymers. Ideally, this polymerization scheme would form flat, ordered arrays. We shall show that, while aggregation can be assuaged by judicious chemical modification of the ribbon edges, GNRs formed when the precursor polymers are oxidized in solution will still tend to aggregate and coil. This will result in kinetically or thermodynamically trapped coils that cannot be expected to effectively flatten when placed on a substrate. If, instead, the oxidation step is performed on the substrate itself, our hypothesis is that aggregation and coiling will be much less of a problem. One complicating factor that we have found, poly(o-phenylenes) tend to form helical secondary structures that also may affect the final conformational state of the GNR on a substrate. We will also provide as-yet unreported details of the helical secondary structures of poly(o-phenylenes) and aspects of colloidal stabilization specifically fabricated in this manner. These computational studies will contribute to the community's understanding of preferential processing routes that would otherwise be difficult to evaluate using experimental methods. It helps to bridge the divide between atomic-scale representation of GNRs and a practical route to recommendations for their physical nanomanufacture.

Paulette Clancy is the Samuel W. and Diane M. Bodman Professor of Chemical and Biomolecular Engineering, Cornell. She is the inaugural Director of the Cornell Institute for Computational Science and Engineering and an Associate Director of the Energy Institute. A native of London, England, she was educated at London and Oxford Universities and joined the faculty in 1987. Her research laboratory studies atomic-scale modeling of semiconductor materials using techniques from ab initio to Molecular Dynamics and Kinetic Monte Carlo. Increasingly, the materials studied by the group have been related to organic and hybrid inorganic-organic semiconductor materials processing. Her team focuses on establishing a link between materials design and properties, suggesting optimized processing conditions and materials discovery to fulfill desired constraints. Throughout her career, she has actively advocated for an increased representation of women among physical scientists and engineers. She is a member of Cornell's Diversity Board and was the inaugural chair of a women faculty committee in Engineering (WISE). The "Women in Nanoscience" (WiN) Fb/Twitter/Blog that she created was set up to encourage women to choose a science career. She has won numerous national and local awards for mentoring and advising students and faculty. http://clancygroup.cbe.cornell.edu/

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