Department of Chemistry and Molecular Biology
Candidate Seminar
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Simulations of Self-assembled Soft Materials: DNA Adsorbents on Metallic and Carbon Nanotube Surfaces.

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Abstract

Assembling inorganic and bio-molecular building blocks into hybrid nano-scale composites holds the potential to yield novel multifunctional materials with tantalizing applications ranging from electronics to medicine. To accelerate the completion of their proof-of-concept development stage, studies of structure-property relationships of hybrid materials are needed. While scanning tunneling microscopy (STM) reveals the structure and electronic transport, theoretical guidance provides understanding of the relationship between measured electronic properties and physical structure of these hybrid materials. We use a combination of density functional theory (DFT) with classical force field calculations to predict and explain STM results on morphology and transport properties of several bio/inorganic composites: DNA strands absorbed on the metallic surface and on the carbon nanotube. For adsorbed DNA molecules on the metallic surface, the use of STM offers the alternative low-cost gene sequencing based on electronic differentiation of DNA bases. Our calculations suggest that unique electronic features, sharp peaks in the *dI/dV* spectra, capable of being measured by STM exist for all four types of DNA bases. The calculated energy of such peaks well agrees with recent dI/dV STM measurements of guanine/Cu samples. For DNA strands wrapped around carbon nanotubes, our simulations reveal a strong relationship between chiral tube coordinates and the wrapping geometry of DNA/nanotube hybrids. Wrapping of the DNA in accordance with the tube's chiral angle provides very stable hybrid systems with wrapping parameters that agree with STM topographic images. Overall, our results provide additional physical insights into the self-assembling mechanisms of bio/inorganic composites.