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Computational characterization of DNA/peptide/nanotube self assembly for bioenergy applications VANESSA ORTIZ, RURIKO ARAKI, GALEN COLLIER, Department of Chemical Engineering, Columbia University — Multi-enzyme pathways have become a subject of increasing interest for their role in the engineering of biomimetic systems for applications including biosensors, bioelectronics, and bioenergy. The efficiencies found in natural metabolic pathways partially arise from biomolecular self-assembly of the component enzymes in an effort to avoid transport limitations. The ultimate goal of this effort is to design and build biofuel cells with efficiencies similar to those of native systems by introducing biomimetic structures that immobilize multiple enzymes in specific orientations on a bioelectrode. To achieve site-specific immobilization, the specificity of DNA-binding domains is exploited with an approach that allows any redox enzyme to be modified to site-specifically bind to double stranded (ds) DNA while retaining activity. Because of its many desirable properties, the bioelectrode of choice is single-wall carbon nanotubes (SWNTs), but little is known about dsDNA/SWNT assembly and how this might affect the activity of the DNA-binding domains. Here we evaluate the feasibility of the proposed assembly by performing atomistic molecular dynamics simulations to look at the stability and conformations adopted by dsDNA when bound to a SWNT. We also evaluate the effects of the presence of a SWNT on the stability of the complex formed by a DNA-binding domain and DNA.

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