# New Method for the Prediction of Carbon Nanostructures and the Application Towards Optimizing Electron Transfer Rates in Dye Sensitized Solar Cells

Liao, Bailey

Dye Sensitized Solar Cells (DSSC) offer a cost-effective means of transforming solar energy into electricity, providing a vast array of applications and a potential solution to our global energy crisis. Current DSSCs utilize titanium dioxide (TiO2) as a semiconducting material to absorb excited electrons. While TiO2 is capable of rapid electron transfer rates, it also exhibits high rates of recombination between electron and electron hole, limiting its efficiency. To this end, I investigated the effectiveness of carbon nanotube structures towards enhancing the efficiency of DSSCs. Primary objectives of this work included: (1) the implementation of graph theory for the prediction of carbon nanostructures and (2) the application of specific carbon nanostructures for the enhancement of electron transfer rates in dye sensitized solar cells. A novel computer program, the Accelerated Topological Annealing of Carbon (ATAC) was modified using mathematical expressions to introduce perfect matching (a fundamental property of graph theory) into the code for the purpose nanostructure prediction. Subsequently, predicted structures were incorporated into both Interfacial Electron Transfer (IET) and Charge Transfer (CT) programs to assess electron transfer rates and effective charge separation. Results demonstrate one structure, a 6,5 nanotube, yielded both increased electron transfer rates and decreased recombination, demonstrating a notable improvement over current DSSC technology. With combinatorial methods of improved nanostructure prediction coupled to both IET and CT evaluation, I propose a method for the high-throughput analysis of carbon nanostructures as a time-saving and cost-efficient alternative to costly DSSC testing.

**Awards Won:**
Fourth Award of $500