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Theoretical Studies of Transport within Single Walled Carbon Nanotubes PAUL MALDONADO, HERNAN MARTINEZ, California State University, Dominguez Hills — Carbon nanotubes have exciting electrical and mechanical properties that seem attractive for ionic and non-ionic transport. However, some fundamental questions about this transport are still not completely understood. One of these questions is how the ion transported through the nanotube is affected by the force and electric fields of the nanotube due to its size and charge. For this investigation to be done, a theoretical structure for a (5,5) single walled carbon nanotube (SWCN) is created by optimizing the geometry of a (5,5) SWCN using semi-empirical PM3 methods. With that optimized structure, computer simulations are performed based on Molecular and Brownian Dynamics techniques to analyze the diffusion through the SWCN. We calculate diffusion coefficients, mean square displacement as well as concentration profiles for both ionic and non-ionic particles moving through them.

Paul Maldonado
California State University, Dominguez Hills

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