Molecular Dynamics Simulations of Methanol in Single-Walled Carbon Nanotubes (SWNTs)

Molecular Dynamics Simulation is an extremely powerful method which involves solving problems in contexts relevant to the study of matter at the atomic level. It is a technique where the time evolution of the molecular system is followed by integrating their equations of motion providing the actual trajectory of the system. The simulation allows the prediction of the static and dynamic properties of substances directly from the underlying interactions between the atoms. The scope of this research is to determine the effect of a "nitrogen defect" has on a methanol molecule encapsulated inside a Single-Walled Carbon Nanotube (SWNT) using molecular visualization programs. The output from classical molecular dynamics simulations were used to investigate the dynamics and behavior of Methanol (CH_3OH) in SWNTs. At the start of all the simulations, methanol is placed near the defect nitrogen in an open nanotube and the system is simulated at various temperatures. In broadest sense, it is difficult to detect and determine the properties of molecules inside nanotubes therefore computational methods such as molecular dynamics simulations were applied to determine the thermal properties of atoms inside the carbon nanotubes. At low temperatures, the methanol molecule remains inside the nanotubes having low diffusion rate. However as the temperature rises, it starts to vibrate and rotate with varying arrays of motion. At 2500 K and above, the molecule completely diffuses out of the carbon nanotube in a spiral manner. These results predict the specific temperature and rate the molecule diffuses out of the carbon nanotube. The simulations also indicate the manner and dynamics of the CH_3OH molecule in nanotubes while the quantum calculations determine the minimal energy required for oxidation reduction of chemical changes in SWNTs.

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