Section E2

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The effect of different charge distributions of urea on molecular wire formation in a single walled carbon nanotube via computational approach

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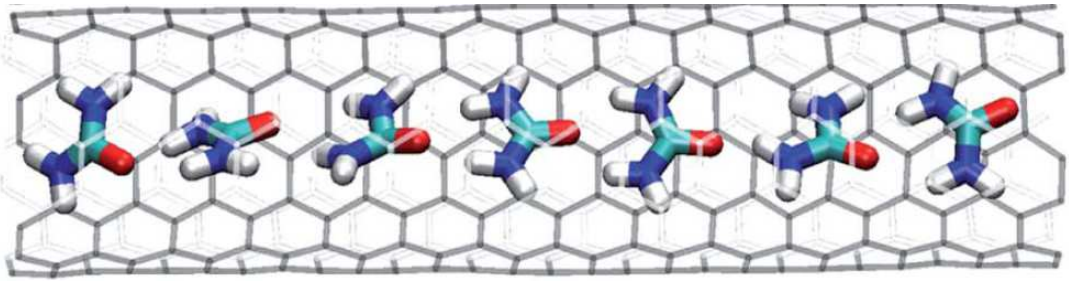
Single walled carbon nanotubes (SWNTs) have a unique size and shape, which leads to the formation of one-dimensional molecular wires when they are immersed in polar solutions. The study of molecular wire formation has many applications in various fields such as drug delivery, water purification, molecular separation, high-flux nano-fluidics devices, signal conversion and many more. The current study incorporated molecular dynamic simulations to investigate how different charge distributions of the urea molecule would affect the molecular wire formation inside of SWNTs. In this study three different charge distributions of urea were studied with neutral armchair type SWNT, and urea models were made by scaling down the charge distribution of KBFF urea. Dipole moments of molecules were affected by the scaled down charge distributions, and the dipole moments of urea-1 (charges scaled down by 1/3), urea-2 (charges scaled down by 2/3) and urea-3 (KBFF urea) molecules were found to be 1.53, 3.06 and 4.60 Debye respectively. Molecular wires were structurally ordered, both translationally and orientationally (as the figure given below), with a contiguous hydrogen bonded network and concerted dipole orientations when urea-1, urea-2 and urea-3 molecules were used, but the difference is the time taken to form the complete urea wire (SWNT with a length of 3.32 nm and a diameter with 0.812 nm forms a 7-membered urea molecular wire).



The flow rates of urea-1 and urea-2 molecules found to be about 9 and 4 times greater than that of urea-3 (KBFF urea) which was found as 0.10 ± 0.04 m s^{-1} and interestingly, interaction energy of adjacent urea molecules follow the inverse order (1 : 4 : ~9). This flow rate difference can be explained by hydrogen bond lifetime of each urea model (0.67, 1.49 and 5.27 ps) and the interaction between two adjacent urea molecules (-3.1, -11.6 and -30.5 kJ mol^{-1}) reside inside the neutral SWNT. The insight gained from this research can be extended to apply SWNT as a drug delivery vehicle and further studies along this line are currently underway.

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