Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Interactions of Carbon Nanotubes with Nitromethane-Water Mixture Governing Selective Adsorption of Energetic Molecules from Aqueous Solution

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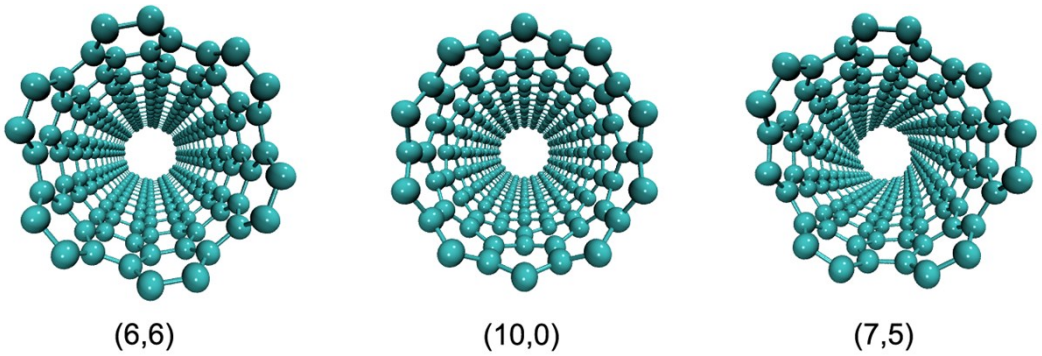

Figure S1 The structures of three SWNTs with similar radii and lengths.

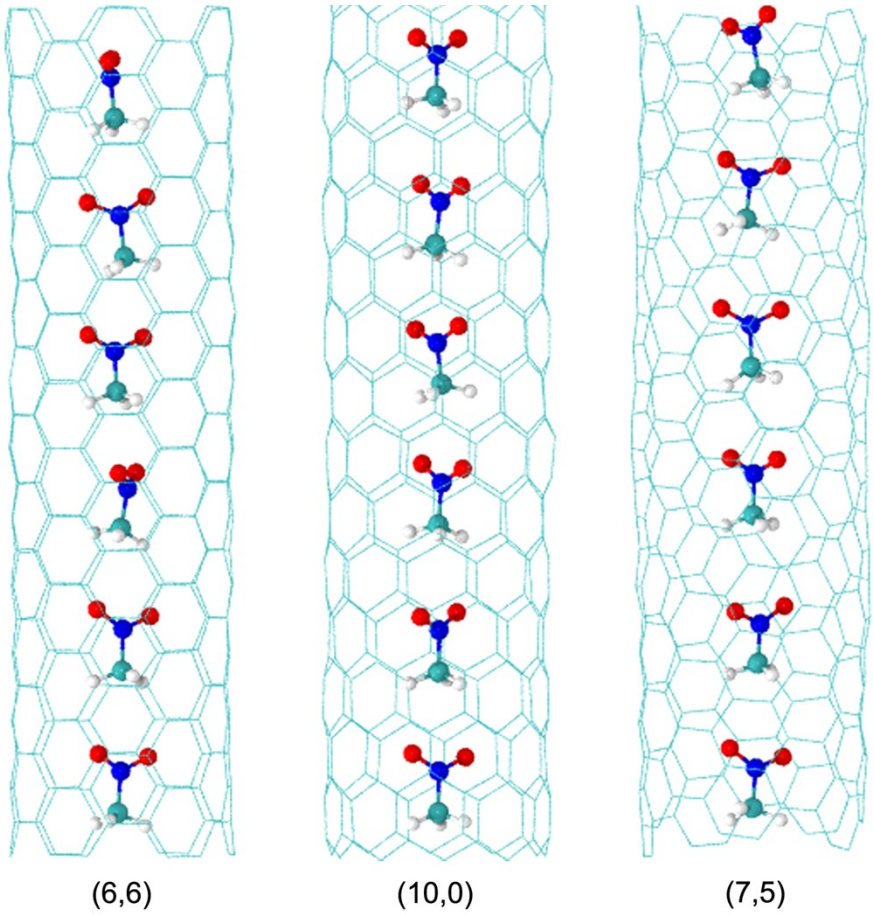

Figure S2 The typical structures of NM adsorbed into the cavities of three SWNTs.

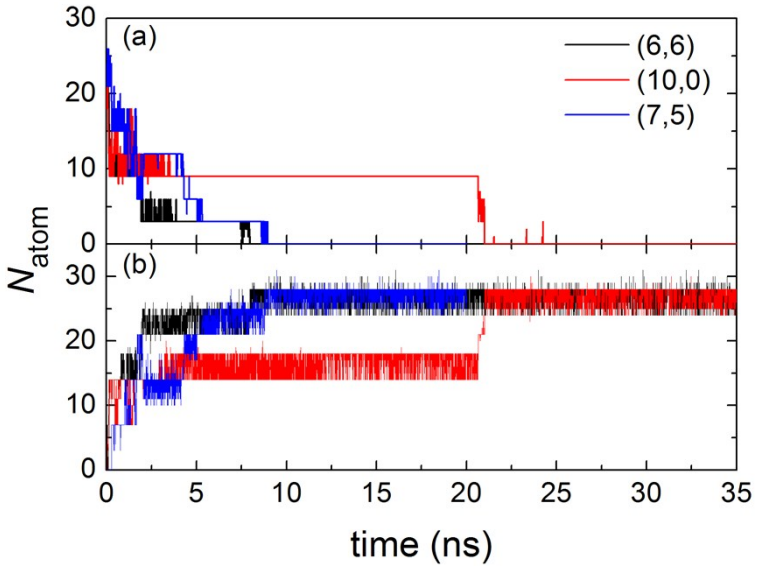

Figure S3. Number of (a) WT and (b) NM atoms inside three SWNTs as a function of simulation time.

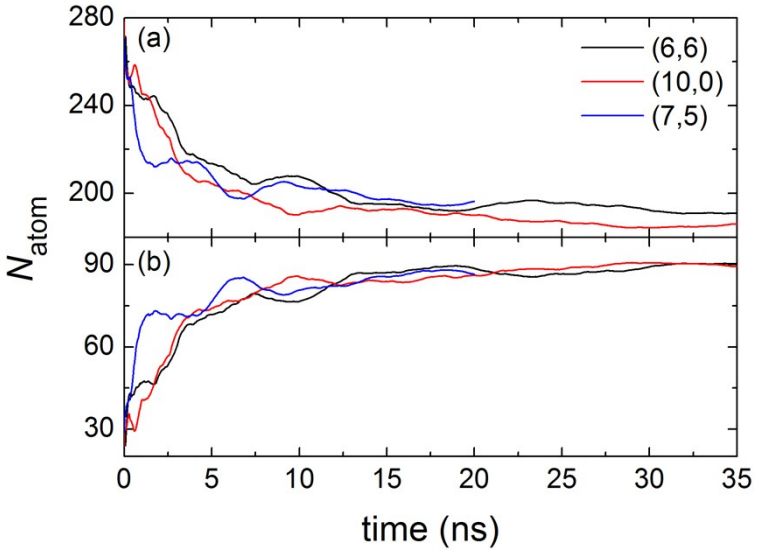

Figure S4. Moving average number of (a) WT and (b) NM atoms within 0.5 nm from the outer wall of three SWNTs as a function of simulation time.