Teeranan Nongnual 2010: Density Functional Theory Evidence for an Electron Hopping Process in Single-Walled Carbon Nanotube-Mediated Redox Reactions. Master of Science (Chemistry), Major Field: Chemistry, Department of Chemistry. Thesis Advisor: Mr. Somkiat Nokbin, Ph.D. 48 pages.

The electron hopping mechanism in the single-walled carbon nanotube (SWCNT)-mediated redox reaction between anthraquinonyl (AQH_2-) and 4-arylhydroxyl amine (4AHA-) groups was studied by density functional theory calculations. The (8,0) SWCNT was used to mimic the real system of interest. It was found that electrons from the oxidized AQH_2 group can be transferred to the oxidizing 4AHA group, at the other end of the nanotube, by a hopping process through the mediating SWCNT. Disparity of electron densities ascribable to non-localized electrons confirmed this finding. The disparity, partial electron density difference, and Hirshfeld partial charges analyses shown that the SWCNT can hold 87% of the extra electron density of the hypothetical negative intermediate produced from the oxidation of the AQH_2 process. Chemical attachments of these two redox reagents to the SWCNT also caused new impurity states within the band gap, thereby giving more metallic characteristics to the system. These findings provided a detailed understanding of the electron hopping process and agree well with a previous experimental study.

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