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Investigation of Chlorophylls a and b Interaction with Inner and Outer Surfaces of Single-Walled Carbon Nanotube Using Molecular Dynamics Simulation

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Abstract : In this work, adsorption of chlorophylls a and b pigments in aqueous solution on the inner and outer surfaces of single-walled carbon nanotube (SWCNT) has been studied using molecular dynamics simulation. The linear interaction energy algorithm has been used to calculate the binding free energy. The results show that the adsorption of two pigments is fine on the both positions. Although there is the close similarity between these two pigments, their interaction with the nanotube is different. This result is useful to separate these pigments from one another. According to interaction energy between the pigments and carbon nanotube, interaction between these pigments-SWCNT on the inner surface is stronger than the outer surface. The interaction of SWCNT with chlorophylls phytol tail is stronger than the interaction of SWCNT with porphyrin ring of chlorophylls.

Keywords : adsorption, chlorophyll, interaction, molecular dynamics simulation, nanotube
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