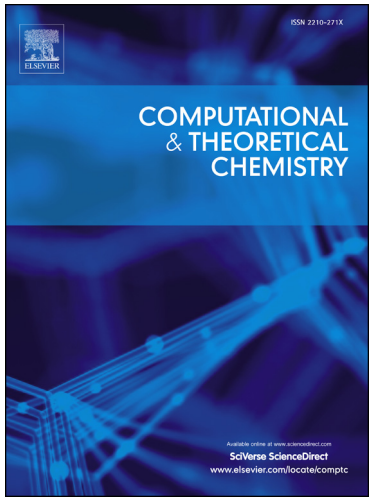

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Molecular Dynamics Simulation of a Cucurbituril Based Molecular Switch Triggered by pH Changes

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Abstract

Molecular Dynamics (MD) Simulations are performed for a cucurbituril-pseudorotaxane system that functions as a molecular switch in which the movement of the macrocycle (CB) component of the rotaxane between two sites is triggered by an appropriate change in pH. The system consists of a CB bead and a fluorenyltriamine string in aqueous solution. Examining the extracted snapshots reveals that the fluorenyl ring bends toward the CB rim when it locates at the butyl moiety, and it becomes aligned with the rest of the guest when it locates at the hexyl moiety. No movement of the macrocycle between the possible positions for CB6 complexes for the fully protonated or the diprotonated guests was observed during the 20 ns simulation. However, such movement was observed in the case of CB7 and CB8. Umbrella sampling was used to obtain the potential of mean force curves, which demonstrates the existence of an energy barrier between the two positions. The height of the barrier was found to decrease as the size of the CB increases. Molecular Mechanics Poisson-Boltzmann Surface Area results indicate that the host-guest electrostatic interactions have the largest contribution to the stability of the complexes.

Keywords: Cucurbit[*n*]uril; Simulations; Molecular switches; MM-PBSA.

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