

Abstract Submitted
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QM/MM and MD study on a light-harvesting molecular triad¹

GUOXIONG SU, ARKADIUSZ CZADER, MARGARET CHEUNG, University of Houston — We investigated the hydrophobic interactions of an artificial photosynthetic molecular triad in nanoconfinement in various sizes using a combined approach of QM/MM method and all-atomistic molecular dynamics simulations with explicit water models. We use the Replica Exchange Method Dynamics (REMD) to investigate the effect of solvation and confinement on the distribution of the ensemble structures and the energy landscape of triad. The relationship of the charge distribution computed from QM/MM and the radial distribution function of water molecules at the proximity of triad will be discussed. The work presented here has profound implications for future studies of the photosynthetic function of triad that provides the opportunity for the insight into the molecular device of green energy.

¹Department of Energy, Basic Energy Sciences (DE-FG02-10ER16175).

Guoxiong Su
University of Houston

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