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Computational studies of energy transfer in dendrimers

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Excited state non-adiabatic molecular dynamics simulations are used to study the nature of the energy transfer in different model dendritic molecules built from linear poly-phenylene ethynylene (PPE) in different architectures. Dendrimers built from these building blocks have been experimentally shown to undergo highly efficient and ultrafast unidirectional energy transfer. We have recently introduced a highly efficient method to compute non-adiabatic excited-state dynamics, including analytically computed gradients and non-adiabatic couplings. The simulations start by an initial vertical excitation selected according to the experimental conditions. By running many simulations, we observe ultrafast and mostly one-directional electronic energy transfer, concomitant with an also ultrafast vibrational energy transfer. The energy gaps and non-adiabatic couplings are strongly influenced by the different nuclear motions in the different potential energy surfaces. This behavior guarantees the successful unidirectional energy transfer associated to the efficient energy funneling in light-harvesting dendrimers.

Prof. Roitberg attended the University of Buenos Aires in Argentina, where he received his Bachelor degree. He attended the University of Illinois at Chicago from 1989 to 1992, where he received his PhD in computational physical chemistry under the direction of Prof. Ron Elber. He was a postdoctoral fellow at Northwestern University from 1992 to 1995, when he moved to the National Institute of Standards and Technology to serve as a staff member. In 2001 he joined the faculty at the university of Florida, in their chemistry and physics departments. He was promoted to Full professor in 2011. Dr. Roitberg is a Fellow of Both ACS and APS and serves now as Chair of the Computers in Chemistry division of ACS..
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