

Abstract Submitted
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Interference of Interchromophoric Energy Transfer Pathways in π -Conjugated Macrocycles TAMMIE NELSON, Los Alamos National Lab, LAURA ALFONSO-HERNANDEZ, Universidad Nacional de Quilmes/CONICET, MAXIM GELIN, Technische Universitat Munchen, JOHN LUPTON, Universitat Regensburg, SERGEI TRETIAK, Los Alamos National Lab, SEBASTIAN FERNANDEZ-ALBERTI, Universidad Nacional de Quilmes/CONICET — The interchromophoric energy transfer pathways between weakly coupled chromophore units in a π -conjugated phenylene-ethynylene macrocycle and its half ring analogue have been investigated using the nonadiabatic excited state molecular dynamics (NA-ESMD) approach. To track the flow of electronic transition density between macrocycle units, we formulate a transition density flux analysis adapted from the statistical minimum flow (SMF) method previously developed to investigate vibrational energy flow. Following photoexcitation, transition density is primarily delocalized on two chromophore units and the system undergoes ultrafast energy transfer creating a localized excited state on a single unit. In the macrocycle, distinct chromophore units donate transition density to a single acceptor unit but do not interchange transition density among each other. We find that energy transfer in the macrocycle is slower than in the corresponding half ring due to the presence of multiple interfering energy transfer pathways. Simulation results are validated by modeling the fluorescence anisotropy decay.

Tammie Nelson
Los Alamos National Lab

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