

Abstract Submitted  
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**Conformational Disorder in Energy Transfer: Beyond Förster Theory** TAMMIE NELSON, Los Alamos National Lab, Los Alamos, New Mexico, SEBASTIAN FERNANDEZ-ALBERTI, Universidad Nacional de Quilmes, Bernal, Argentina, ADRIAN ROITBERG, University of Florida, Gainesville, SERGEI TRETIKOV, Los Alamos National Lab, Los Alamos, New Mexico — Energy transfer in donor/acceptor chromophore pairs, where the absorption of each species is well separated, can be understood through a Förster resonance energy transfer model. The picture is more complex for organic conjugated polymers, where the total absorption spectrum can be described as a sum of the individual contributions from each subunit, whose absorption is not well separated. Although excitations in these systems tend to be well localized, traditional *donors* and *acceptors* cannot be defined and energy transfer can occur through various pathways. In addition, fast torsional motions between individual monomers can break conjugation and lead to reordering of excited state energy levels. Energy transfer in these systems can be induced by both electronic transitions and by fast torsional fluctuations where both mechanisms occur simultaneously. We use non-adiabatic excited state molecular dynamics (NA-ESMD) to simulate energy transfer between two poly-phenylene vinylene (PPV) segments composed of 3-rings and 4-rings separated by varying distances. The transition density decay represents the transfer rate, and can be decomposed into contributions from various transfer pathways.

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