

# **Modeling of photoinduced relaxation pathways in conjugated polymers and carbon nanotubes**

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Prediction and understanding of photoinduced processes in molecular- and nano-materials is fundamental to a myriad of technological applications, ranging from sensing, imaging, solar energy harvesting, to future optoelectronic devices. This talk will overview several applications of recently developed excited state molecular dynamics framework incorporating non-adiabatic quantum transitions studying ultrafast dynamics and exciton transport in several conjugated molecular systems. Our analysis shows intricate details of photoinduced vibronic relaxation and identifies the conformational degrees of freedom leading to ultrafast dynamics and energy transfer. This theoretical modeling allows us to understand and to potentially manipulate energy transfer pathways in molecular materials suitable for solar energy conversion.