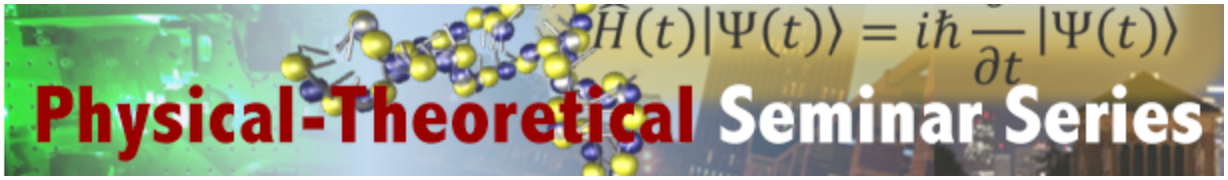

Monday, April 9, 2018, 12:00 pm
Seaver Science Library, Room 150
SSC Auditorium next to the library

Professor Massimo Olivucci

Department of Chemistry
Bowling Green State University

Is Vibrational Coherence Required for Optimizing Double Bond Photoisomerization Quantum Yields?

The quantum yield of a photochemical reaction is one of the most fundamental quantities in photochemistry, as it measures the efficiency of the transduction of light energy into chemical energy at the molecular level. Nature has developed protein cavities able to dramatically amplify the quantum yield of photochemically active chromophores. The retinal chromophore sterically constrained inside the cavity of the dim-light visual pigment rhodopsin represents an outstanding example of such a control. In this contribution, we use non-adiabatic dynamics simulations to investigate the relationship between quantum efficiency and the phase of specific vibrational modes during the light induced coherent dynamics of rhodopsin. We show that such relationship rationalizes a recently observed but counterintuitive dependence of quantum yields from isotope substitutions. We also show that the same relationship can be applied to the computational design of biomimetic optomechanical devices.

References:
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Hosted by Professor Anna Krylov

The scientific community is invited

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