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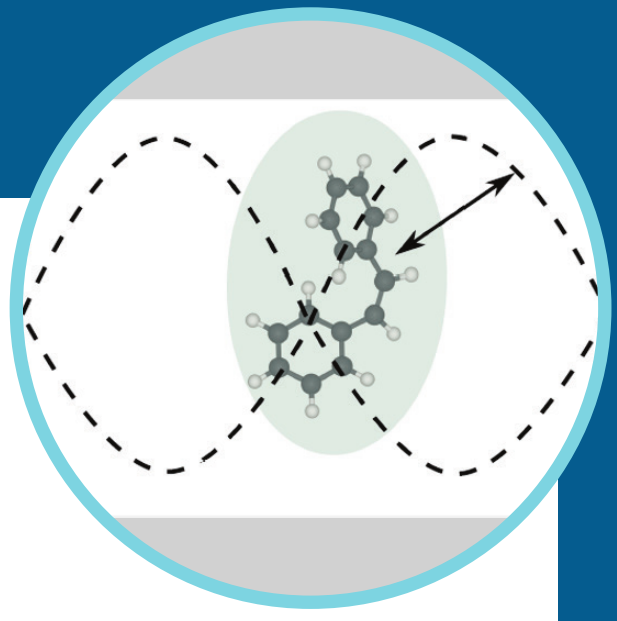
When: Sep 10, at 16:00-17:00
Where: Blue Bldg (TPOC-3), room 408

Energy Colloquium and CMS Seminar

MULTIPLE CLONING AND POLARITONS IN EXCITED STATE NON-ADIABATIC MOLECULAR DYNAMICS

Speaker:
Sergei Tretiak

Center for Energy Science and Technology, Skolkovo Institute of Science and Technology, Russia.
s.tretiak@skolkovotech.ru
faculty.skoltech.ru/people/sergeitretiak



ABSTRACT

Modelling of photoexcited dynamics in extended molecular systems and solids beyond Born Oppenheimer regime is a next frontier of atomistic electronic structure theory. This talk will overview recently developed theoretical methodologies underlying EXcited-state Molecular Dynamics simulations (NEXMD) framework developed at LANL. In particular, I will overview a new implementation of Ab Initio Multiple Cloning (AIMC) method, which is applied for non-adiabatic excited-state molecular dynamics simulations of photoinduced processes in conjugated molecules. The cloning procedure directly affects electronic and vibrational coherence, relaxation and unidirectional energy transfer between dendritic branches. A recent NEXMD capability is modeling of the dynamics of molecules strongly interacting with quantum light. The methodology is exemplified on the cis-trans photoisomerization of a realistic molecule in a cavity. Numerical simulations demonstrate that the photochemical reactions can be controlled by tuning the properties of the cavity. In the calculated example, the isomerization is suppressed when polaritonic states develop a local minimum on the lower polaritonic state. Moreover, the observed reduction of isomerization is tunable via the photon energy and light-molecule coupling strength. These insights suggest quantum control of photochemical reactions is possible by specially designed photonic or plasmonic cavities. Observed relationships between spatial extent/properties of electronic wavefunctions and resulting electronic functionalities allow us to understand and to potentially manipulate excited state dynamics and energy transfer pathways toward optoelectronic applications.

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