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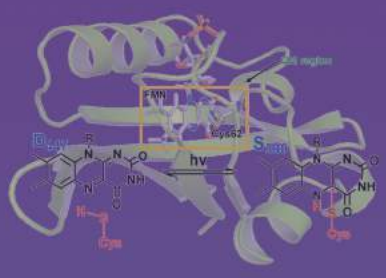


COMPUTATIONAL CHEMISTRY SEMINAR SERIES

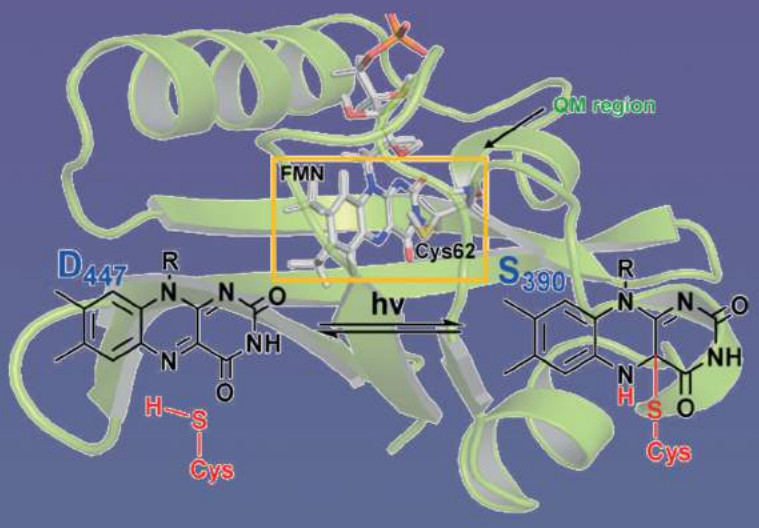
Excited-State Electronic Structures and Nonadiabatic Dynamics of Complex Systems

SPEAKER:
Ganglong Cui, Beijing Normal University

TIME:
2:00pm-3:00pm, Wednesday, April 3, 2019

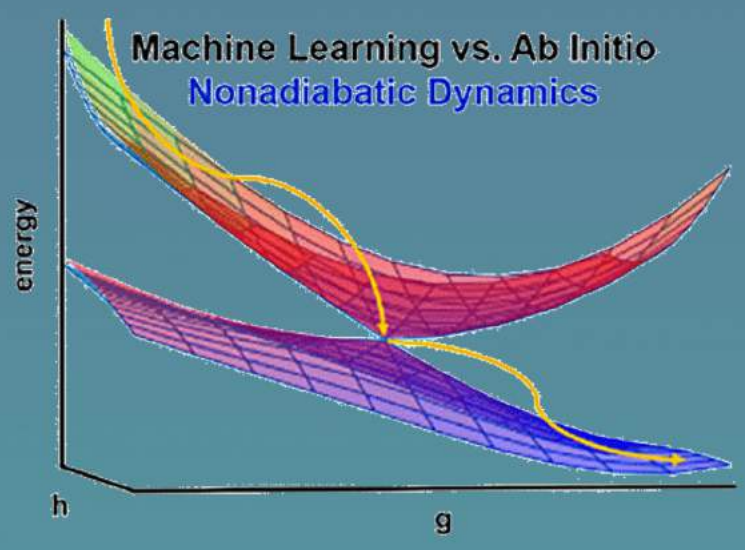
VENUE:
Room 264, Geography Building, Zhongbei Campus, ECNU

HOST:
Xiao He, East China Normal University



Abstract:

Photophysical processes and photochemical reactions are very complicated and widely involved in the fields of chemistry, biology, materials, atmospheric chemistry, etc. Understanding related mechanisms is essentially important for subsequent optimization, control, and design of involved processes. Now it is still difficult to completely understand these details at the atomistic level merely depending on experimental techniques. In this regard, computer simulations have become an important and complementary tool. On the other hand, accurate simulations of complex systems are highly dependent on the developments of efficient excited-state electronic structure and nonadiabatic dynamics methods. In this talk, we will present our recent ab initio excited-state electronic structure calculations on the photophysical and photochemical mechanisms of the dark- and light-adapted states of a blue-light Light-oxygen-voltage (LOV) photoreceptor and some progresses on the development of an initio nonadiabatic dynamics methods and their applications in simulating ultrafast excited-state relaxation dynamics in organometallic systems, etc.



Biography:

Ganglong Cui is currently a Professor of Chemistry at Beijing Normal University. He obtained his joint Ph.D. from Beijing Normal University and Duke University. He then dis his post-doctoral research at Max-Planck-Institut für Kohlenforschung in Germany. As of 2019, he has published more than 90 SCI papers in Nat. Commun., J. Am. Chem. Soc., Angew. Chem. Int. Ed., etc. His research interests lie in methodological developments of excited-state electronic structures and non-adiabatic dynamics; their applications on photoinduced physical and chemical processes in chemistry, biology and materials.