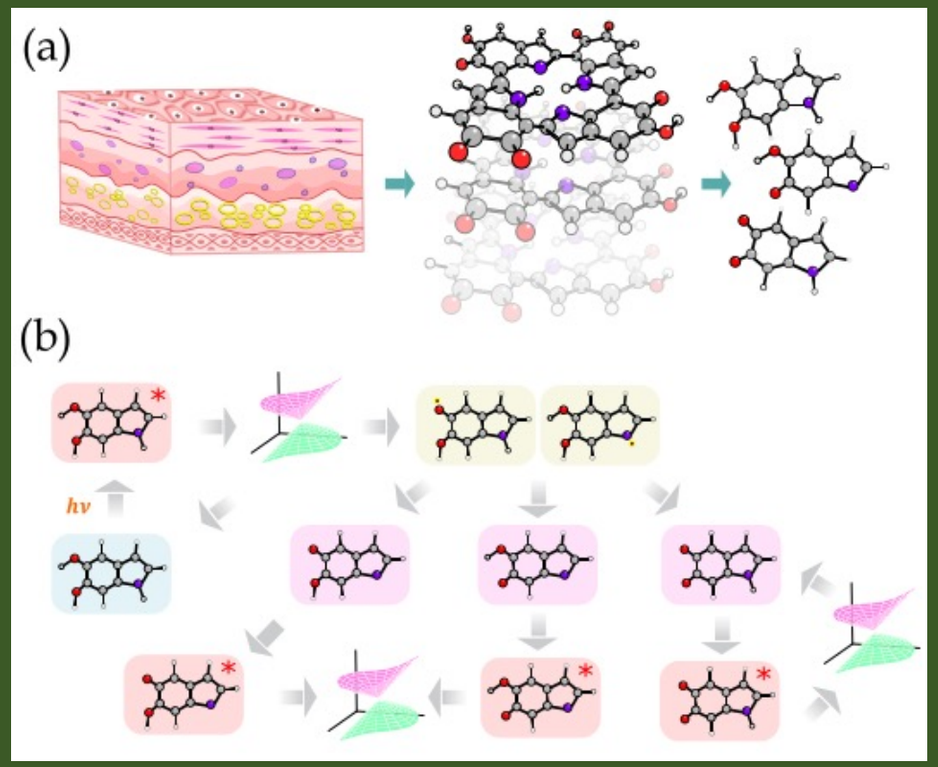
ASET FORUM OF TIFR

Quantum chemistry methods to study strongly correlated systems – from variational to machine learning approaches

Prof. Debashree Ghosh (Indian Association for the Cultivation of Science, Kolkata)



Polyaromatic hydrocarbons (PAHs) such as acenes have long been studied due to its interesting optical properties and low singlet triplet gaps. Earlier studies[1,2] have already noticed that use of complete valence active space is imperative to the understanding of its qualitative and quantitative properties. Since complete active space-based methods cannot be applied to such large active spaces, we have used density matrix renormalization group (DMRG)[3] based approaches. Further small modification to the PAH topology shows interesting new phases of behaviour in its optical gaps. We have understood the effect of these effects based on spin frustration due to the presence of odd membered rings. In this talk, I will discuss these observations from molecular and model Hamiltonian perspectives[4].

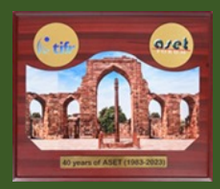
Further developments based on artificial neural network based configuration interaction for strongly correlated systems will also be discussed[5]. The similarities between the ANNs and the MPS wavefunctions will be leveraged for 2D systems.

1. The radical character of the acenes: A density matrix renormalization group study, J. Hachmann, J.J. Dorando, M. Aviles, G.K.-L. Chan, J. Chem. Phys., 127(13), 134309 (2007).
2. Singlet triplet gaps in polyacenes: a delicate balance between static and dynamic correlations investigated by spin flip methods, C.U. Ibeji, D. Ghosh, Phys. Chem. Chem. Phys., 17(15), 9849 (2016).
3. Orbital Optimization in the density matrix renormalization group, with applications to polyenes and beta carotene, D. Ghosh, J. Hachmann, T. Yanai, G. K.-L. Chan, J. Chem. Phys., 128(14), 144117 (2008).
4. In the quest for a stable triplet state in small polyaromatic hydrocarbons: an in silico tool for rational design and prediction, M. Rano, S.K. Ghosh, D. Ghosh, Chemical Science, 10, 9270 (2019).
5. Configuration interaction trained by neural networks : Application to model polyaromatic hydrocarbons, S.K. Ghosh, M. Rano, D. Ghosh, J. Chem. Phys., 154, 094117 (2021).

Debashree Ghosh obtained her M.S. degree in Chemical Sciences from IISc in 2005 and PhD degree from Cornell University, USA in 2010. She joined CSIR-NCL as a Senior Scientist in 2012, subsequently moving to Indian Association for the Cultivation of Science. Currently, she is a professor at the School of Chemical Sciences in IACS. Her research focuses on the development of polarizable force fields and their hybrid frameworks with excited-state electronic structure methods, geared towards understanding the photo-physics of biological systems. She has been recognized by several awards, including the Annual Medal of the International Academy of Quantum Molecular Science (2021), SERB-POWER fellowship (2022) and Walter Kohn prize awarded by International Centre for Theoretical Physics (2022).

Friday, December 1, 2023 at 4 p.m.

Hybrid: Lecture Theatre AG 66, ***YouTube Live: https://tinyurl.com/ASETon1Dec***



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