北京大学量子材料科学中心

International Center for Quantum Materials, PKU

Seminar

Towards the Fundamental Design of Hydrogen-Bond Networks as Fluorescent Optical Probes

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Time: 10:00 am, Jan.26, 2026 (Monday)

时间：2026年1月26日 （周一）上午10:00

Venue: Room w563, Physics building, Peking University

地点：北京大学物理楼，西563会议室

Abstract

Fluorescence takes place throughout the nature world. Most conventional chemical wisdom proposes that in organic molecules, fluorescence occurs in conjugated systems, such as in the aromatics. However, in most biological contexts, the interaction of light with matter occurs in media built up of dense networks of hydrogen bonds (HBNs). Recent experiments suggest that is also possible to observe fluorescence from these networks although the electronic and nuclear components that leads to this emergent phenomena remains an open question. Being able to use these HBNs has the possibility of opening up enormous practical potential paving the way for the design of non-invasive probes.

My talk will be focused on challenging our intuitions on the physics and chemistry behind the notion of a *fluorophore.* By combining both experiments and state-of-the-art electronic structure and molecular dynamics simulations, I will elucidate our attempts to decipher the origins of intrinsic fluorescence [1,2,3,4]. Certain chemistries that form supramolecular assemblies lend themselves to the formation of more stiff HBNs sometimes leading to proton transfer and the rigidification of vibrational modes both of which can inhibit non-radiative decay. We demonstrate this for a wide class of systems ranging from amyloid proteins to different amino-acids including Glutamine, Cysteine and Lysine.

I will then move on to discussing unpublished work looking at the photophysics and chemistry of aqueous systems including Ice and Liquid Water. If the phenomena of HBN fluorescence is more general, what are the conditions that modulate the photoexcitation and subsequent photochemistry in aqueous solutions. I will discuss recent work on examining the role of topological and ionic defects in modulating the optical properties of Ice [5] and in Liquid Water.

[1] https://pubs.acs.org/doi/10.1021/jacs.5b11012
[2] https://www.pnas.org/doi/10.1073/pnas.2020389118
[3] https://www.nature.com/articles/s41467-023-42874-3
[4] https://onlinelibrary.wiley.com/doi/full/10.1002/anie.202505331
[5] https://arxiv.org/abs/2506.16568

About the speaker

Ali A. Hassanali is a Full Professor at the International Centre for Theoretical Physics (ICTP). He obtained a PhD in 2010 at The Ohio State University and finished the postdoc in 2013 at ETH-Z and USI-Lugano. His research is at the boundary between physics, chemistry, and biology. He is interested in the physical chemistry of aqueous systems. He and his group used advanced computational techniques, including both classical and first principles electronic structure approaches, to investigate the structural, dynamical, electronic, and optical properties of organic matter immersed in water. He has published around 90 research papers, including several in Science, Nature Communications, and PNAS journals. Ali was awarded an ERC Proof of Concept Grant, EuroExascale Supercomputing Award, Prestigous ERC Consolidator Grant, co-PI, DARPA Grant, HORIZON 2020, FET Open Grant, KAUST Supercomputing grant, etc.