PhD THESIS DEFENSE - Excitons in Motion: Linking Structure and Transport in Energy Materials

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10:00
ICFO Auditorium

The growing global energy demand, coupled with the need to reduce CO2 emissions, highlights the urgency of developing sustainable energy solutions. Despite its vast potential, solar energy remains underutilized due to technological challenges. Most solar technologies- including photovoltaics (PV), concentrated solar power, and artificial photosynthesis- depend on three core processes: light absorption, energy conversion, and energy transport. Understanding how light is converted and transmitted- primarily via exciton diffusion- in materials ranging from semiconductors to biomimetic and biological systems is essential for improving the performance of both optoelectronic devices and natural photosynthesis.

This thesis examines how dimensionality, defects, and molecular geometry affect exciton diffusion, aiming to uncover structure-function relationships that govern energy transport in energy-related materials. Using advanced spatiotemporal microscopy - including Time-Correlated Single-Photon Counting Microscopy, Transient Reflection Microscopy, and a novel technique developed by my group, Structured Excitation Energy Transfer (StrEET) - this research investigates exciton diffusion in organic semiconductors, 2D perovskites, transition metal dichalcogenides (TMDCs), and bio-inspired systems.

Key findings show that dimensionality critically influences exciton mobility. In Y6 organic films - a leading non-fullerene acceptor for organic photovoltaics - I performed the first direct measurements of exciton diffusion, revealing that confinement enhances mobility. Combined with morphological tuning via additives, diffusion coefficients increase by over 50%. In 2D perovskites, increasing thickness boosts both diffusion and anisotropy, yielding diffusion lengths well beyond those of conventional organic systems.

TMDC studies reveal that, beyond dimensionality, defects and substrate interactions significantly affect exciton mobility. In suspended monolayers, multiple transport regimes - rapid, negative, and slow diffusion - are observed, each constrained by trap states and sensitive to structural and environmental changes.

Lastly, this work explores how molecular packing and geometry influence exciton transport in bio-inspired systems like porphyrin films and bacterial LH2 networks. Using the novel highly sensitive StrEET technique, I conducted the first direct measurements of exciton transport in photosynthetic systems. Denser molecular packing enhances diffusion while reducing exciton lifetimes; the optimal diffusion length, comparable to that of top organic semiconductors, arises from a balance between these competing effects, offering insights into the design of artificial light-harvesting systems.

Overall, this research demonstrates that excitonic transport can be engineered by tuning material properties such as dimensionality, defect density, and molecular organization. These findings provide guiding principles for developing more efficient optoelectronic and bio-inspired energy technologies, supporting the transition to sustainable energy solutions.

Friday June 27, 10:00 h. ICFO Auditorium
Thesis Director: Prof. Dr. Niek Van Hulst
Hosted by: Prof. Dr. Niek Van Hulst