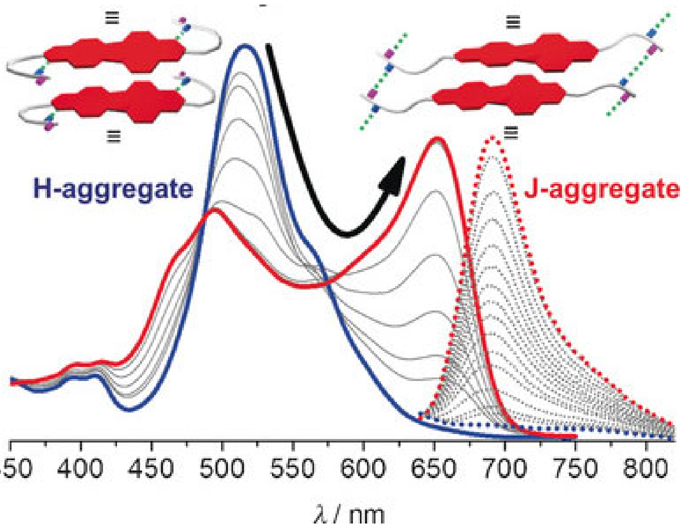
Title	Optimizing chromophores aggregation for Enhanced Light Harvesting
PI	Marcella Bonchio
Research Group	NANOMOLCAT
Curriculum	Scienze Chimiche
Location	DiSC
Contact	web: https://nanomolcat.wixsite.com/nanomolcat
	email: marcella.bonchio@unipd.it

Project description:

The surge in interest in conjugated organic materials for display technology and photovoltaics has spurred research into understanding electronic excitations in organic molecular assemblies. Achieving optimal performance necessitates efficient design strategies considering molecular dyes, sample morphology, and intermolecular interactions, particularly aggregation phenomena like J- and H-aggregates, pivotal for optoelectronic device applications. This Ph.D. project aims to advance organic optoelectronics by focusing on designing and forming stable H and J-aggregates of perylene bisimides (PBIs) in water-based environments, building on prior research that developed the "artificial Quantasome." The candidate will investigate strategies to control PBI aggregation from H-type to J-type, enhancing light-harvesting for efficient energy transfer in optoelectronic devices.

Two main strategies will be pursued: i) **Rational Design of Novel PBIs for Stable J-Aggregates**: Synthesizing PBIs with specific substituents in bay positions inspired by chlorosome design principles, influencing absorption spectra, dipole interactions, and hydrogen bonding. Exploring modifications to PBI molecular structures to enhance J-aggregate formation efficiency and stability. ii) **Aggregation Control over PBIs Assembly**: Synthesizing PBIs to regulate aggregation from H-type to J-type through ion interactions, investigating conditions promoting one aggregation type over the other and understanding interaction stability and reversibility.



The project, highly interdisciplinary, integrates organic chromophore synthesis with state-of-the-art techniques such as NMR, FT-IR, Raman, photophysical characterization (Absorption, Emission, Circular Dichroism, Cyclic Voltammetry), supramolecular studies (DLS, Z-Potential, Powder X-Ray Diffraction PXRD), and computational investigations to better understand specific interactions.

This research holds promise for advancing organic optoelectronics, offering insights into efficient light-harvesting and energy transfer processes, critical for future optoelectronic device development.

Publications: M. Bonchio et al, Chemistry–A European Journal, 2024, e202303784, M. Bonchio et al., Journal of the American Chemical Society, 2022, 144 (31), 14021-14025, M. Bonchio et al. Nature Chemistry, 2019, 11 (2), 146-153