THEORETICAL MODELING OF SQUARAINE AGGREGATES AND THIN FILMS

Squaraine aggregates and thin films are widely studied organic chromophores with unique spectral properties, making them ideal for engineering functional molecules in fields like organic optoelectronics, bioimaging, xerography, and photodynamic therapy.

In this seminar, two case studies will explore the intriguing properties of squaraine aggregates and thin films from a theoretical perspective. The first study utilizes an essential state model (ESM) to investigate how disorder and intermolecular charge transfer (ICT) affect the chiroptical properties of chiral aggregates of proline-derived anilino squaraines with varying terminal alkyl chain lengths. The second study applies the ESM approach to elucidate the mechanism of photoinduced charge separation in single-component films of a near-IR squaraine dye.

Dr. Davide Giavazzi received the M.S. in Chemistry from the University of Parma and the Ph.D. in Materials Science and Technology in 2024, under the supervision of Prof. Anna Painelli. He is currently a postdoctoral researcher at the University of Parma. His research focuses on theoretical spectroscopy of molecular aggregates and organic functional materials and on quantum dynamical approaches to describe relaxation processes in molecular and supramolecular systems.

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WEDNESDAY, OCT. 23
1:00 PM - 2:20 PM
Tiernan Lecture Hall I

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