Molecular Materials & Modeling (M3)

webpage: under construction

Elenco dei componenti del gruppo con relativa e-mail:
Referente: Lidia Armelao (lidia.armelao@unipd.it).
Componenti: Gregorio Bottaro (gregorio.bottaro@unipd.it); Silvia Carlotto (silvia.carlotto@unipd.it); Daniel Forrer (daniel.forrer@unipd.it); Marta Maria Natile (martamaria.natile@unipd.it); Marzio Rancan (marzio.rancan@unipd.it); Andrea Vittadini (andrea.vittadini@unipd.it)

The Molecular Materials & Modeling (M3) Group is composed of researchers belonging to the Department of Chemical Sciences of the University of Padova and of the Institute for Condensed Matter Chemistry and Technologies for Energy (ICMATE) of the National Research Council (CNR). The group activity is currently focusing on the design, synthesis, characterization, and modeling of supramolecular structures and of nanocrystalline inorganic solids with applications in energy, nanomedicine, sensing, and catalysis. Innovative molecular systems and inorganic nanostructures are obtained through strategies of molecular self-assembly by exploiting non-covalent, selective, and directional interactions. All the

systems are studied and characterized with advanced experimental techniques and computational methods.

Riferimenti bibliografici recenti e rappresentativi:

- Adaptive helicity and chiral recognition in bright europium quadruple-stranded helicates induced by host-guest interaction. *Cell Rep. Phys. Sci.* **2022**, 3, 100692.
- Chromium doped $ZnGa_2O_4$ thin films: an X-ray Absorption Near Edge Structure (XANES) and X-ray Excited Optical Luminesce (XEOL) study. *Appl. Surf. Sci.* **2022**, 577, 151896.
- Spatial and temporal resolution of luminescence quenching in small up-conversion nanocrystals. *ACS Appl. Mater. Interfaces* **2022**, 14, 11883−11894.
- Nature of the ligand-centered triplet state in Gd^{3+} β-diketonate complexes as revealed by time-resolved EPR spectroscopy and DFT calculations. *Inorg. Chem.* **2021**, 60,15141−15150.
- Digging Ti interstitials at the r-TiO_2 (110) surface: mechanism of porphyrin Ti sequestration by iminic N nucleophilic attack. *Appl. Surf. Sci.* **2021**, 564, 150403.
- Luminescent thermometers: from a library of europium (III) β-diketonates to a general model for predicting the thermometric behavior of europium-based coordination systems. *ChemPhotoChem* **2020**, 4, 674−684.