

## THE STATUS OF THE RESEARCH ACTIVITIES IN THE LaSCAMM AT THE UNIVERSITY OF BASILICATA

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We will briefly outline the main research activities that have been performed in this last year in our research group also in collaboration with other Italian research groups of the same university (prof. C. Bonini, Prof. C. Minichino, Prof. G. Ricciardi) and of other universities (Prof. F. Devillanova, Prof. M. Ghedini, Prof. G. Resnati).

Our main goal in this few years have been focused on the study of molecular system and their interactions for the understanding and development of molecular systems for application in light-matter interactions.

In this field we have focused our attention both on elementary processes related to the single molecule process, on the interaction that arise using particularly tailored molecules and on some catalytic processes for asymmetric synthesis. The subject of our studies using DFT and post-Hartree-Fock methods are related to

- elementary intramolecular processes leading luminescence
- elementary processes for photo-dynamic therapy
- Intramolecular vibrational relaxation of excited states
- Role of relativistic effects on UV-Vis spectroscopy of heavy metal complexes
- Kinetics of excited states
- Interpretations of weak interactions in the so called "Halogen Bond"
- Heavy halogen interaction with chalcogen containing molecules
- Role of alkaline metals in catalytic processes ring opening in enantiotropic synthesis

Further aspects related to thermodynamic behaviour of nano-structure materials containing macro-cyclic coordination complexes with discotic structure leading to mesogen phases have been tackled by means of Molecular Dynamics approach.

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1. M. Amati, D. Casarini, F. Lelej *Journal of American Chemical Society* in preparation
2. P. Cristinziano, F. Lelej *Journal of Chemical Physics* in preparation
3. C. Minichino, M. Amati, F. Lelej *Chem Phys. Lett* to be submitted; *Journal of Chemical Physics* in preparation
4. P. Romaniello, F. Lelej, M. Arca, Francesco A. Devillanova; *Chemical Physics Physical Chemistry*, *submitted*
5. M. La Deda, A. Grisolia, I. Aiello, A. Crispini, M. Ghedini, S. Belviso, M. Amati, F. Lelej; *Journal of the Chemical Society, Dalton Transactions*, *submitted*
6. M. C. Aragoni, M. Arca, F. Demartin, F. A. Devillanova, F. Lelej, P. Grimaldi, F. Isaia, V. Lippolis, A. Mancini, L. Pala, G. Verani; *Journal of the Chemical Society, Dalton Transactions in press*
7. M. Amati, F. Lelej, R. Liantonio, P. Metrangolo, S. Luzzati, T. Pilati, G. Resnati; *J. Fluorine Chem. In press*
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