

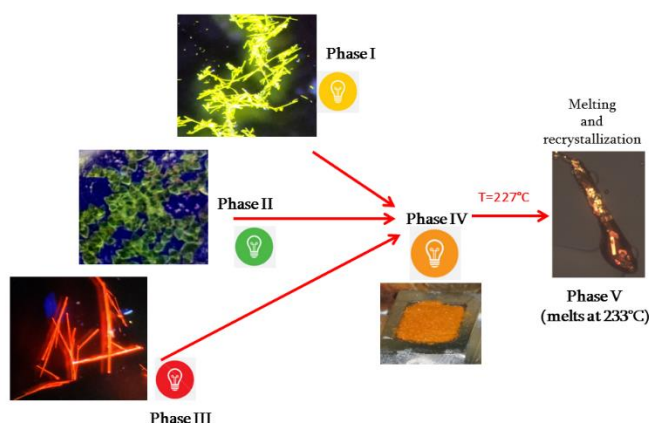


Prof. Lucia Maini

Dipartimento di Chimica "G. Ciamician"
Università di Bologna
Via Selmi 2
l.maini@unibo.it

One molecule, four colours, discovering the polymorphs of thieno(bis)imide derivatives by single crystal and powder X-ray diffraction

2,3-Thieno(bis)imide (TBI) based materials are emerging as valuable molecular materials for application in organic electronics thanks to their ambipolar charge transport properties combined to tunable electroluminescence. This new class of materials is being tested as active layer in thin films organic devices, such as ambipolar light emitting transistors (OLETs), field-effect transistors (OFETs) and both as donor and acceptors in photovoltaic cells (OPV). These molecules often present different crystalline modifications which show different photo-physical properties. One of these molecules, named NTA[1], shows a strong tendency to form different polymorphs. Until now we have observed at least four different crystalline phases, each one characterized by a particular colour, emission under UV light and crystals morphology. The crystal structure of form II and form III was obtained by single crystal x-rays diffraction; while form I and IV were characterized by powder diffraction. The main interaction that drives the crystallization is the π -stacking between the aromatic cores of the molecules, forming channels possibly suitable for the charge transport. The form III seems to be the most appropriate for the charge transport due to the packing of the molecules that form columnar stack linked together through π - π interactions.



[1] M. Zambianchi, L. Favaretto, M. Durso, C. Bettini, A. Zanelli, I. Manet, M. Gazzano, L. Maini, D. Gentili, S. Toffanin, F. Gallino, M. Muccini, M. Cavallini, and M. Melucci, *J. Mater. Chem. C*, 2015, 3, 121.