"Threaded molecular wires as model conjugated polymers with controlled interstrand interactions"

Franco Cacialli

Department of Physics and Astronomy, and London Centre for Nanotechnology, University College London, Gower Street, WC1E 6BT, London, UK
Tel + 44 20 7679 4467, f.cacialli@ucl.ac.uk

Threaded molecular wires[1] made with conjugated-polymers-based polyrotaxanes offer an example of a "bottom-up" approach to electroluminescent nanostructures. An attractive feature is that this class of materials is engineered at a supramolecular level by threading a conjugated macromolecule, such as poly(*para*-phenylene), poly(4,4'-diphenylene vinylene) or poly(9,9'-fluorene) through α- or β-cyclodextrin rings, so as to reduce intermolecular interactions and solid-state packing effects, that red-shift and partially quench the luminescence. Such a supramolecular approach preserves the fundamental semiconducting properties of the conjugated wires, and is effective at both increasing the photoluminescence efficiency and blue-shifting the emission of the conjugated cores, in the solid state, while still allowing charge-transport. We used the polymers to prepare single-layer light-emitting diodes with Ca and Al cathodes, and observed blue and green emission. The reduced tendency for polymer chains to aggregate shows in both solid-state films, as well as in solution (as clearly demonstrated by the study of fluorescence decay via time-correlated single-photon counting experiments) and allows solution-processing of individual polyrotaxane wires onto substrates, as revealed by scanning-force microscopy[1]. Control of the threading ratio is possible, thereby resulting in fine tuning of the excitonic vs aggregate contribution to the luminescence, as well as of the electro- and photo-luminescence efficiency[2].

1. F. Cacialli, J.S. Wilson, J. J. Michels, C. Daniel, C. Silva, R. H. Friend, N. Severin, P. Samorì, J. P. Rabe, M. J. O'Connell, P. N. Taylor, H. L. Anderson. "Cyclodextrin-threaded conjugated polyrotaxanes as electroluminescent insulated molecular wires with reduced interstrand interactions". *Nature Materials*. **1**, 160-164 (2002).
2. S Brovelli, G. Latini, M. J. Frampton, S. O. McDonnel, F. Oddy, O. Fenwick, H. L. Anderson and F. Cacialli. "Enhanced electroluminescence of threaded molecular wires via fine tuning of their threading ratio". *Nano Letters.* **8**, 4546-4551 (2008).