Thermo-, solvato- and mechanochromism in mononuclear Cu(I) emitters is governed by a common mechanism.

G. A. Filonenko, Department of Chemical Engineering, Delft University of Technology

Photoluminescent (PL) properties of coordination compounds in the solid state are nearly impossible to predict. This essential challenge stems from the complexity of the emission phenomena in the solid state and the lack of adequate computational tools that could assist us in making accurate predictions. On this background, making the PL of coordination compounds responsive to external stimuli is even more challenging as it requires control over a virtually unpredictable property.

Stimuli-responsive PL complexes, however, exist despite these limitations. Such compounds change their emission colour in response to variations of temperature, pressure and external mechanical force. The mechanism governing these changes in PL behaviour is unknown and a large part of responsive emitters were typically designed through trial and error until recently. A recent pioneering work suggested that variations in interaction strength between cationic and anionic parts of the emissive complex are the major cause for the stimuli response in Cu(I) emitters. Our work demonstrates that this, in fact, is a general phenomenon.

In this work we describe a series of simple mononuclear Cu(I) complexes that show pronounced thermochromism in crystalline, amorphous and solution state. We link this thermochromic behaviour to the variations in cation/anion separation in these complexes. To probe this hypothesis we designed an emitter where both charge carriers of the same compound were bound to separate polymer chains that would allow to induce charge separation mechanically rather than thermally. Strikingly, this reference system showed pronounced mechanochromism in addition to thermochromic behaviour. These findings have multiple implications: on one hand they show that control over charge separation is indeed a potent general PL tuning strategy, on the other hand our data clearly demonstrates that thermal and mechanical phenomena in polymer mechanochemistry are interlinked.


E-mail G.A.Filonenko@tudelft.nl