

ABSTRACT

The PhD Thesis entitled "*Silica nanoparticles as inorganic scaffolds for the preparation of hybrid materials for the optical detection of anions*" deals with the combination of supramolecular and material chemistry concepts to prepare hybrid sensing materials with the ability to detect selected ions through color and emission changes.

The first hybrid material prepared is based in the use of silica nanoparticles as inorganic scaffold functionalized with spirobenzopyrans (signaling unit) and with thiourea moieties (binding unit). In the final nanoparticles the spirobenzopyran signaling unit is in its open polar conformation (red color merocyanine structure). Coordination of long chain carboxylates (octanoate, decanoate and dodecanoate) with the thiourea moieties induced the formation of a dense hydrophobic monolayer around the signaling unit. This non-polar monolayer induced a change in the conformation of the spirobenzopyran to the closed spirocyclic form with a subsequent color change.

The second part of this PhD Thesis was related with the preparation of silica nanoparticles functionalized with anthracene, as signalling subunit, and two different thioureas, as anion binding sites. Acetonitrile suspensions of the bifunctionalized nanoparticles showed the typical structured emission band of the anthracene fluorophore. Addition of certain anions to acetonitrile suspensions of the nanoparticles induced

an enhancement of the emission intensity (Cl^- , Br^- , H_2PO_4^- , acetate and benzoate) or a marked quenching (F^- and CN^-).

Finally, the last part of this PhD Thesis deals with the preparation of silica nanoparticles functionalized with terpyridine binding sites and sulforhodamine B as signaling subunit. Coordination of transition metal cations (Fe^{3+} , Hg^{2+} , Cu^{2+} , Ni^{2+} and Pb^{2+}) with the terpyridine binding sites induced a marked quenching of the emission intensity (ca. 95%) of the sulforhodamine B fluorophore. The prepared materials were used for the fluorogenic recognition of anions. At this respect, addition of H_2PO_4^- , HSO_4^- , F^- , Cl^- , Br^- , I^- and NO_3^- anions induced different degrees of cation displacements with the subsequent enhancement of the emission intensity of the fluorophore. Principal component analysis (PCA) allowed the discrimination of all the anions tested. Besides, only H_2PO_4^- anion was able to induce the displacement of Pb^{2+} cation with the subsequent emission enhancement.