Journal of Chemical Sciences

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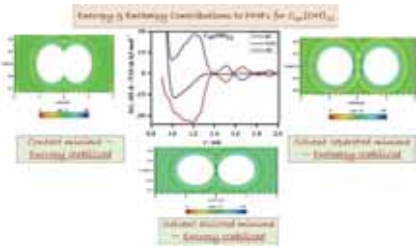
Regular Article



Aqueous solutions of fullerene derivatives have found applications in molecular sensing devices, biochemistry and environmental science. Therefore, it is necessary to have a microscopic understanding of the solvation structure of such macromolecules. Association and dynamics of fullerene and fullerols [$C_{60}(OH)_n$] in water are addressed by molecular dynamics simulations.

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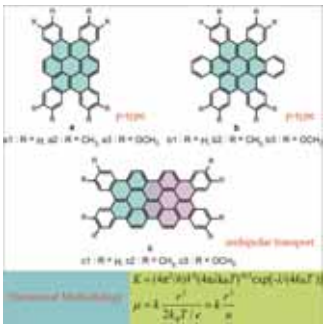

Density functional theory was used to compute the charge transport rates of three series of nine coronene topological structures at the M06-2X/6–31+G(d) level. Tetrabenzocoronene (series a) and hexabenzocoronene (series b) could be candidates for a hole-transporting (p-type) organic semiconductor material, and 'long plate-like' coronene topological structures (series c) could be used as an ambipolar transport material.

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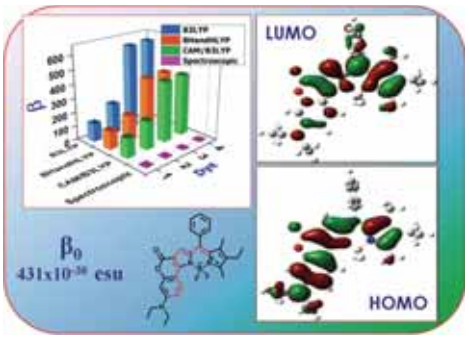

The NLO properties of coumarin-fused BODIPY hybrid chromophores were studied in detail. Spectroscopic method gave rough estimation of polarizability and hyperpolarizability characteristics of four hybrid chromophores while computational approaches using three different hybrid functionals, B3LYP, CAM-B3LYP and BHandHLYP in combination with 6-311+G(d,p) basis set, gave comparative estimation of these values. BLA/BOA calculations for ground and excited states suggested that the cyanine-type D-π-A framework produces high NLO response. The hybrid molecules are proven to be the better performing NLOphores than the isolated coumarin or BODIPY units.

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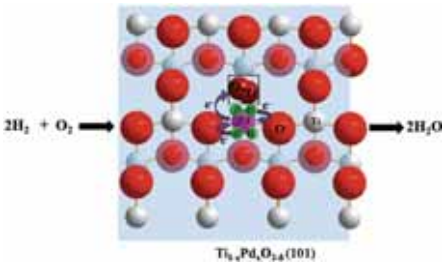

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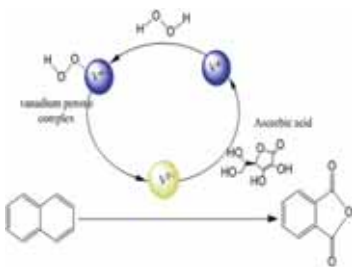

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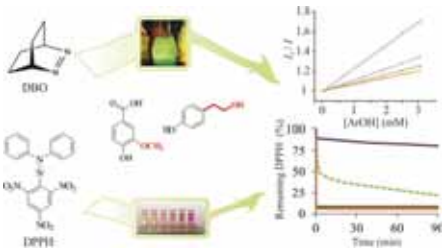

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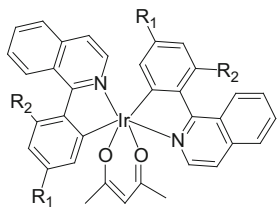

R_1=H, R_2=H
R_1 = F, R_2=F
R_1=CF_3, R_2=H
R_1=$N(CH_3)_2$, R_2=H
R_1 = $COCH_3$, R_2=H

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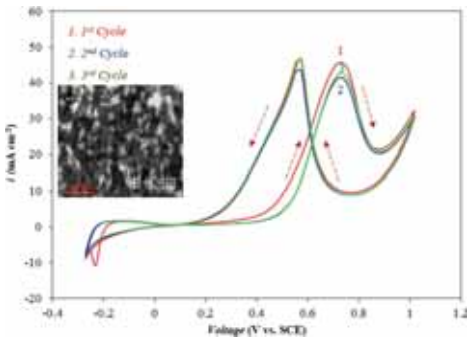

Electrochemical investigation of electrodeposited platinum nanoparticles on multi walled carbon nanotubes for methanol electro-oxidation

Electrodeposition of platinum nanoparticles (PtNPs) on multiwall carbon nanotubes (MWCNTs)/flourine-doped tin oxide glass (FTO) was conducted successfully. The electrodeposition mechanism of PtNPs nucleation and growth on MWCNTs was studied. It was found that fine and well-distributed PtNPs/MWCNTs electrode shows a high electrochemical activity for methanol electro-oxidation.

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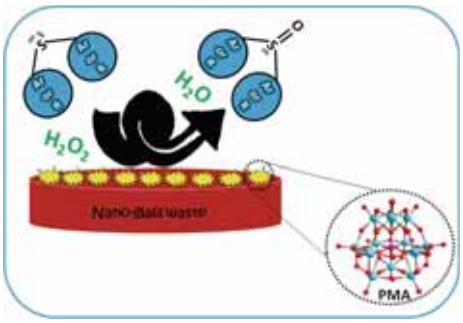

Nano-sized glass as an economically viable and eco-benign support to anchor heteropolyacids for green and sustainable chemoselective oxidation of sulfides to sulfoxides

Nano-glass waste-supported phosphomolybdic acid (n-GW/PMA) was synthesized as a novel, highly efficient and retrievable nanocatalyst for the chemoselective, green and rapid oxidation of sulfides to sulfoxides through an experimental design (CCD) approach. The prepared catalyst was characterized by FT-IR, TGA, XRD, FE-SEM and EDX techniques.

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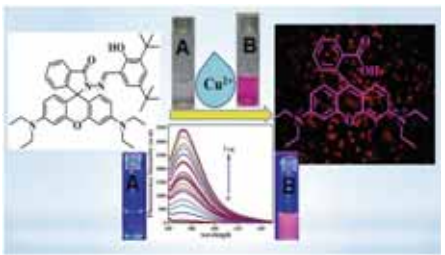

A new rhodamine based 'turn-on' Cu^{2+} ion selective chemosensor in aqueous system applicable in bioimaging

A new 'turn-on' non-cytotoxic rhodamine hydrazone derivative (**L**) senses Cu^{2+} ion in nano molar region selectively in 20 mM HEPES buffer [pH 7.4; water/acetonitrile (9:1 v/v)] and is an efficient biomarker to detect Cu^{2+} ions in living cells.

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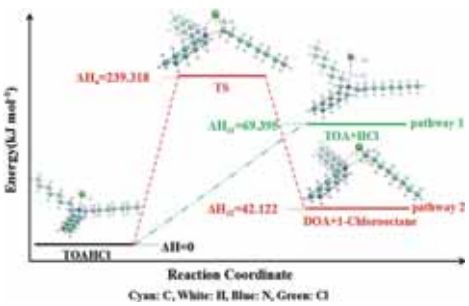

Mechanism studies on thermal dissociation of tri-n-octylamine hydrochloride with FTIR, TG, DSC and quantum chemical methods

The thermal dissociation of tri-n-octylamine hydrochloride was investigated with both the quantum chemical simulation and experimental methods. Intrinsic reaction coordinate (IRC) calculations suggest that the products are tri-n-octylamine and HCl rather than di-n-octylamine and 1-chlorooctane. Furthermore, the dissociation is a two-stage process as determined by experimental analysis.

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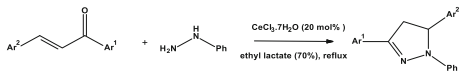

A facile protocol for the synthesis of 1,3,5-triaryl-2-pyrazolines is described. The solvent ethyl lactate, obtained from renewable sources, is biodegradable. The catalyst $CeCl_3 \cdot 7H_2O$ is a water-tolerant Lewis acid with low toxicity. Easy and clean work up, recyclable solvent and catalyst are the merits of the protocol. The reaction works well for all systems giving good yields of the desired products.

Regular Article

A novel tandem Betti/Ullmann/oxidation reaction was introduced for synthesis of new oxazepine derivatives. This method provides a new and useful strategy for the construction of heterocycles. In this regard, Fe_3O_4@SiO_2-boric acid nanoparticles have been synthesized and used for the synthesis of desired novel Betti bases based on kojic acid derivatives.

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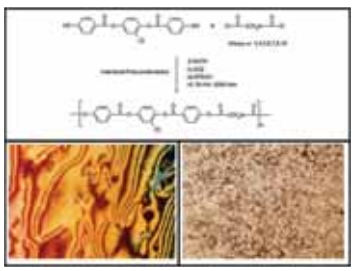

The present study deals with the synthesis of thermotropic liquid crystalline polyesters derived from bis[4-hydroxy benzoyloxy]-2-chloro-1,4-benzene (BHBOCB) and aliphatic dicarboxylic acid chlorides by interfacial polycondensation methodology.

Regular Article

An eco-friendly method was used to synthesise three oxyma-sulfonate esters using two-phase (dichloromethane-water) method in presence of sodium carbonate for scavenging HCl. The oxyma sulfonate esters were characterized using different spectroscopic techniques (FT-IR, NMR, UV-Vis) as well as X-ray single crystal diffraction analysis. The electronic and spectroscopic properties of these esters were computed using DFT/B3LYP method.

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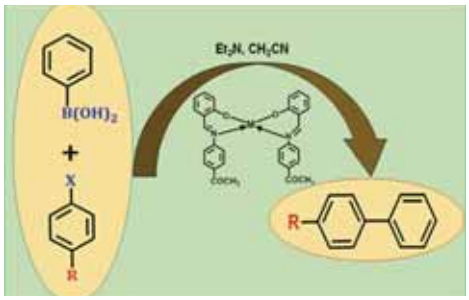

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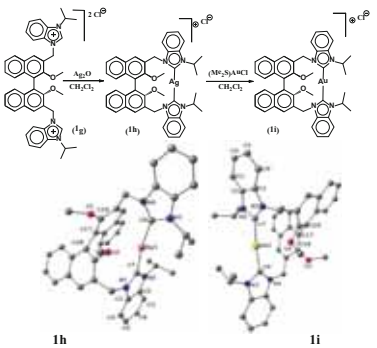

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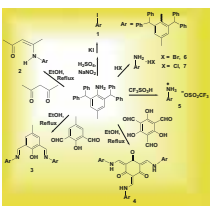

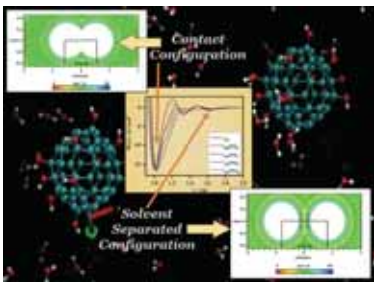

Cover picture: Potentials of mean force between the COMs of C_{60}, $C_{60}(OH)_2$, $C_{60}(OH)_4$, $C_{60}(OH)_8$, and $C_{60}(OH)_{12}$ in water.
For details, see the paper by Sonanki Keshri and B L Tembe (pp. 1327–1340)

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