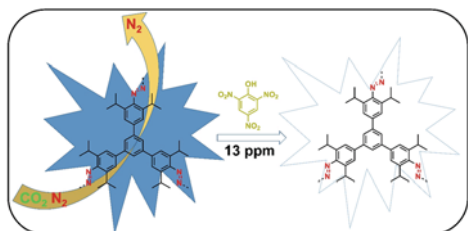


## CONTENTS

### Regular Article

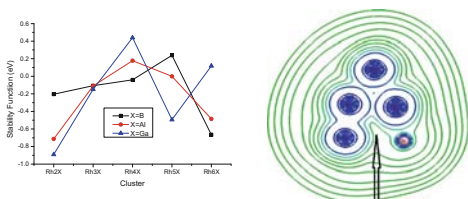


**Picric acid sensing and CO<sub>2</sub> capture by a sterically encumbered azo-linked fluorescent triphenylbenzene based covalent organic polymer**

Dhananjayan Kaleeswaran and Ramaswamy Murugavel . . . . . 1

Sterically encumbered azo-linked covalent organic polymer (*i*PrTAPB-Azo-COP) has been synthesized from a fluorescent hexaisopropyl substituted triphenylbenzene platform. The resulting fluorescent porous COP has been utilized for picric acid sensing and CO<sub>2</sub> capture.

### Regular Article

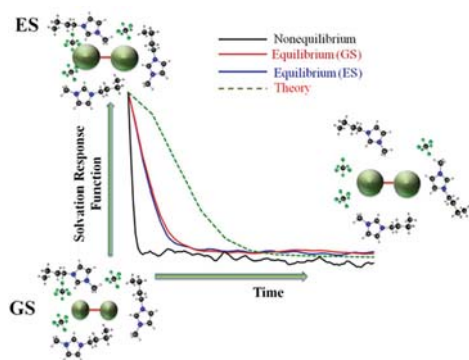


**Density functional theory study of structure, electronic and magnetic properties of non-metal (Group 13) doped stable Rh<sub>n</sub> (n = 2–8) clusters and their catalytic activities towards methanol activation**

Abhijit Dutta and Paritosh Mondal . . . . . 2

In this study, B or Al or Ga is incorporated into pure rhodium clusters to evaluate the structural, electronic and magnetic properties using density functional theory. Structural and electronic parameters reveal the higher stability of Rh<sub>5</sub>B, Rh<sub>4</sub>, Al and Rh<sub>4</sub>Ga clusters. Also, these doped clusters show methanol activation.

### Regular Article



**Nonpolar solvation dynamics for a nonpolar solute in room temperature ionic liquid: a nonequilibrium molecular dynamics simulation study**

Sandipa Indra and Snehasis Daschakraborty . . . . . 3

Nonpolar solvation dynamics of a nondipolar solute probe in an imidazolium ionic liquid has been studied using classical molecular dynamics simulation method. The equilibrium and non-equilibrium simulated solvation response functions have been compared with experimentally measured (using 3PEPS) and theoretically predicted (using mode coupling based theory) solvation response function. The study reveals that the experimental solvation timescales can originate from the purely nonpolar interaction between excited solute and ionic liquid solvent molecules.

## Regular Article

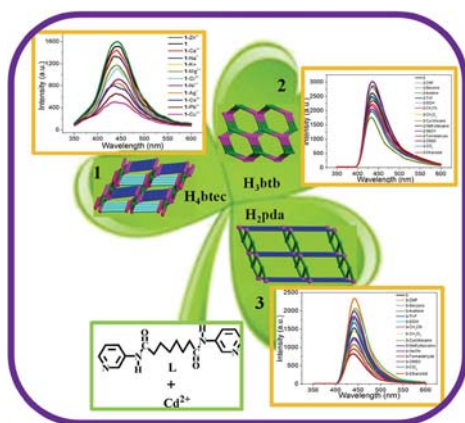


### Gold nanodots self-assembled polyelectrolyte film as reusable catalyst for reduction of nitroaromatics

Perumal Viswanathan and Ramasamy Ramaraj . . . . .4

Colloidal gold nanoparticles are efficient catalysts for organic reactions. But the removal of homogeneous gold colloids from the reaction mixture is very difficult. To address this issue, gold nanodots were synthesized and self-assembled over polyelectrolyte film to form catalytic plates. Removal of these reusable catalytic plates from the reaction mixture is facile.

## Regular Article

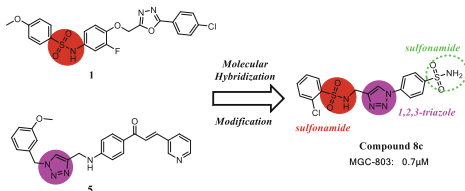


### Effect of three aromatic polycarboxylates on the structural diversities and properties of three new cadmium(II) coordination compounds

Hongyan Lin, Jiafeng Lin, Jing Zhao, Yuan Tian, Xiang Wang and Guocheng Liu. . . . .5

Three new Cd(II) coordination compounds based on the flexible bis(pyridyl)-bis(amide) ligand and three different polycarboxylates have been hydrothermally synthesized. The polycarboxylates with diverse carboxyl groups and various structures play an important role in constructing three Cd(II) compounds. The thermal stabilities, fluorescent and fluorescence sensing properties of the three Cd(II) compounds towards small solvent molecules and metal cations have been reported.

## Regular Article

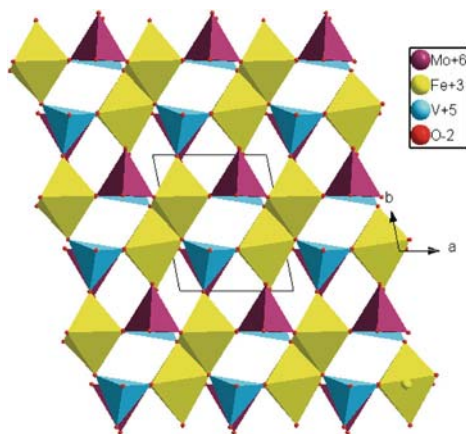


### Efficient click reaction towards novel sulfonamide hybrids by molecular hybridization strategy as antiproliferative agents

Dong-Jun Fu, Yu-Hui Hou, Sai-Yang Zhang and Yan-Bing Zhang . . . 6

Twelve novel sulfonamide hybrids were designed by molecular hybridization strategy. These sulfonamide hybrids were synthesized by click reaction and evaluated for their antiproliferative activity. Among them, compound **8c** showed potent antiproliferative activity with an  $IC_{50}$  value of 0.7  $\mu\text{mol}$  against MGC-803 cells.

## Regular Article

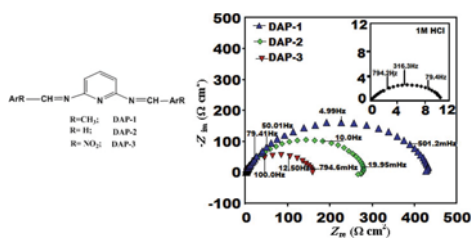


### Electrochemical study of two structurally related compounds FeVMoO<sub>7</sub> and CrVMoO<sub>7</sub> synthesized by sol-gel method

D Saritha . . . . .7

FeVMoO<sub>7</sub> and CrVMoO<sub>7</sub> phases have been studied as electrode materials for the first time. Sol-gel method was adopted, for the first time, to synthesize these phases and the phases exhibit good electrochemical behavior. Electrochemical lithium insertion into three dimensional phases of FeVMoO<sub>7</sub> and CrVMoO<sub>7</sub> is feasible and good cycling behavior was observed.

Regular Article

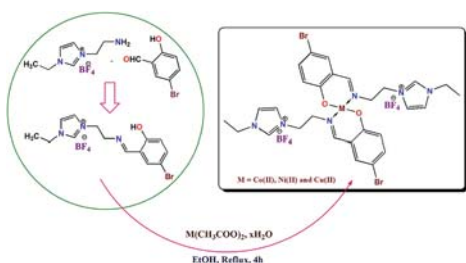


**A combined electrochemical and theoretical study of pyridine-based Schiff bases as novel corrosion inhibitors for mild steel in hydrochloric acid medium**

Parul Dohare, M A Quraishi and I B Obot . . . . .8

Three pyridine-based Schiff bases were synthesized, characterized, and their corrosion inhibition performance was studied on mild steel in 1 M HCl solution. Results of gravimetric measurements, potentiodynamic polarization, EIS, and SEM, AFM image analyses are reported. The inhibitor molecules follow Langmuir isotherm and showed mixed-type behavior. Experimental results were supported by DFT calculations and Monte Carlo simulations.

Regular Article

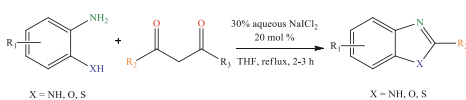


**Physico-chemical characterization and biological studies of newly synthesized metal complexes of an Ionic liquid-supported Schiff base: 1-{2-[(2-hydroxy-5-bromobenzylidene)amino]ethyl}-3-ethylimidazolium tetrafluoroborate**

Sanjoy Saha, Goutam Basak and Biswajit Sinha . . . . .9

Co(II), Ni(II) and Cu(II) complexes bearing an ionic liquid-supported Schiff base 1-{2-[(2-hydroxy-5-bromobenzylidene)amino]ethyl}-3-ethylimidazolium tetrafluoroborate as ligand, is reported. The spectral and magnetic susceptibility measurements suggest that the bidentate ligand coordinates to the central metal ion through the azomethine nitrogen and phenolic oxygen atoms, yielding a square planar complex.

Regular Article

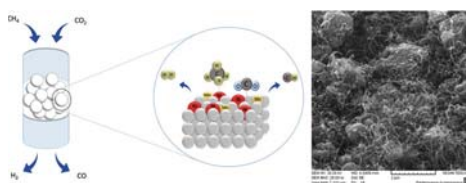


**Sodium dichloroiodate promoted C-C bond cleavage: An efficient synthesis of 1,3-Benzazoles via condensation of *o*-amino/mercaptan/hydroxyanilines with  $\beta$ -diketones**

Saket B Bhagat, Shrikant M Ghodse and Vikas N Telvekar . . . . .10

A facile protocol has been developed for the synthesis of three versatile 1,3-benzazoles *viz* 2-substituted 1*H*-benzimidazoles, benzoxazoles and benzothiazoles from readily available starting materials, 1,3-diketones and corresponding *o*-amino anilines/thiophenols/phenols, by aqueous sodium dichloroiodate (NaIO<sub>3</sub>) mediated C—C bond cleavage. The reaction provides a rapid access to these 1, 3-benzazoles in good yields, thus speeding up the drug discovery process.

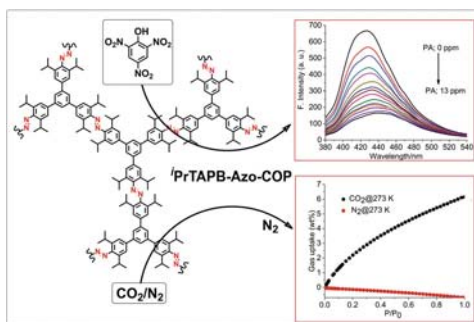
Regular Article



**Preparation and evaluation of mesoporous nickel and manganese bimetallic nanocatalysts in methane dry reforming process for syngas production**

Yalda Ramezani, Fereshteh Meshkani and Mehran Rezaei . . . . .11

Promotional role of Mn in bimetallic Ni-Mn catalyst supported on mesoporous nanocrystalline  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> leads to strong interaction between the support and the active metal, which causes high activity and stability with no severe coke deposition compared to the monometallic sample.



Cover picture: Picric acid sensing and  $\text{CO}_2$  capture by a sterically encumbered azolinked fluorescent triphenylbenzene based covalent organic polymer. For details, see the paper by Dhananjayan Kaleeswaran and Ramaswamy Murugavel. (Article ID: 1)