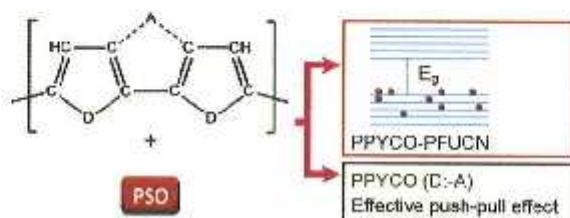


CONTENTS

- 9 **Designing of novel donor-acceptor-donor framework based low band gap copolymers using an artificial intelligence approach**

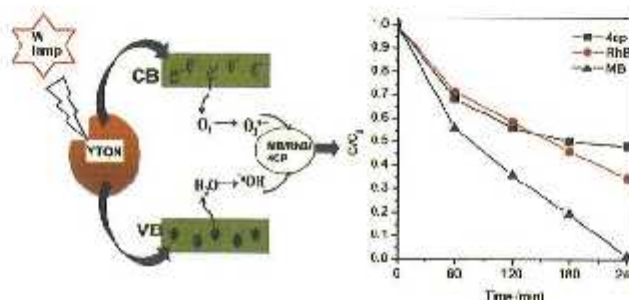
Novel binary D-A-D copolymers have been designed using the PSO algorithm. The donor moieties considered are thiophene, pyrrole and furan with $>C-(CN)_2$ and $>C=O$ acceptor groups. A higher relative percentage of PPYCO in a copolymer is highly desirable for designing low E_g materials. PPYCO-PFUCN copolymer is found to have the lowest band gap.



Priyanka Thakral & A K Bakshi*

- 20 **Synthesis of $Y_2Ti_2O_7-xN_x$ with visible light responsive photocatalytic activity**

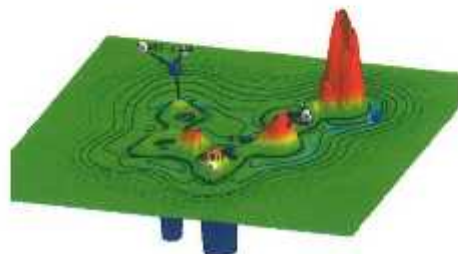
Nitrogen doped $Y_2Ti_2O_7$ is prepared by a facile solid state method using urea as a source of nitrogen. It is a visible light responsive photocatalyst and degrades organic pollutants such as methylene blue, rhodamine B and 4-chlorophenol under visible light irradiation.



G Ravi, Saleh Mansouri, Suresh Palla & M Vithal*

- 27 **Ultrafast radiationless decay mechanisms through conical intersections in cytosine: Computational insight and topological analysis of the charge density distributions**

Contour plots and relief maps have been analyzed for regions of valence shell charge concentrations and depletions in the ground state and the two CI structures of cytosine. NBO analysis reveals that the conformational and overall stability of the studied cytosine conformations are facilitated by the competitive conjugative and the lone-pair interactions.

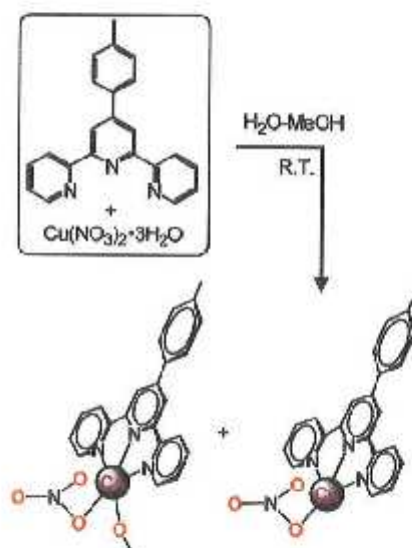


Rifaat Hilal^a, Saadallah G Aziz, Abdulrahman O Alyoubi & Shaaban A Elroby

Notes

- 35 **A two-component co-crystal of Cu(II) complex of *p*-tolyl-terpyridine**

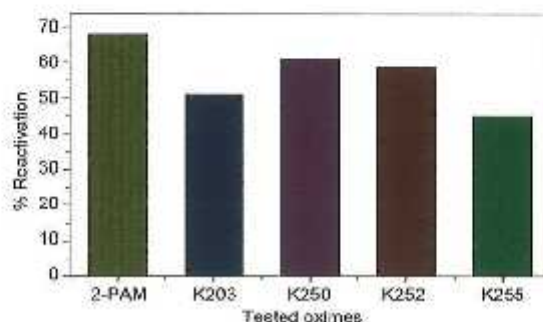
The two-component co-crystal, $[\text{Cu}(\text{L})(\text{NO}_3)_2][\text{Cu}(\text{L})(\text{NO}_3)(\text{CH}_3\text{OH})(\text{NO}_3) \cdot \text{H}_2\text{O}]$ ($\text{L} = p$ -tolyl-terpyridine) crystallizes in the triclinic system (space group $P\bar{1}$) and comprises two mononuclear Cu(II) moieties, one cationic and the other neutral. While one of the Cu(II) centres furnishes a five-coordinated distorted square pyramidal geometry (CuN_3O_2), the other Cu(II) centre displays a four-coordinate distorted square planar geometry (CuN_3O).



- 40 **Kinetic and physicochemical analysis of structurally different bis-pyridinium oximes against pesticide inhibited AChE**

The effect of functional group on the second pyridinium ring of bis-pyridinium oximes for the reactivation of paraoxon inhibited AChE is studied. Reactivation studies show that K250 is the most efficient reactivator among all the investigated oximes, although it could not surpass the reactivity of standard oximes against paraoxon.

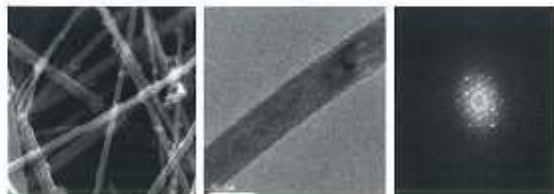
Arvind Kumar Sahu, Bhanushree Gupta,
Rahul Sharma, Yama Singh, Kamil Musilek,
Kamil Kuca & Kallol K Ghosh*



- 46 **Synthesis of β -MnO₂ nanowires and their electrochemical capacitive behavior**

Well-defined γ -MnOOH and β -MnO₂ nanowires are synthesised using hydrothermal process. The synthesized γ -MnOOH nanowires are transformed to β -MnO₂ nanowires (20-30 nm in width and >5 μ m in length) which show nearly three times higher specific capacitance (404 F/g) as compared to commercial grade MnO₂. The present synthesis process indicates that β -MnO₂ can be prepared in large scale.

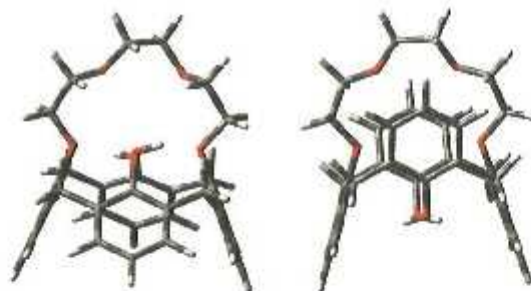
Indra B Singh* & So-Moon Park



- 52 **Influence of hydrogen bonding on the conformational stability of calix[4]crown-4 ether**

Influence of non-covalent interactions on the conformational stability of calix[4]crown-4 ether is investigated using various quantum mechanical methods. The relative stability of the conformers follows the order: zone > partial cone > 1,3-alternate.

Satish Kumar*, KM Mathew, Neelam, P R Sahoo &
Arun Kumar



- 59 **Guide to Authors**