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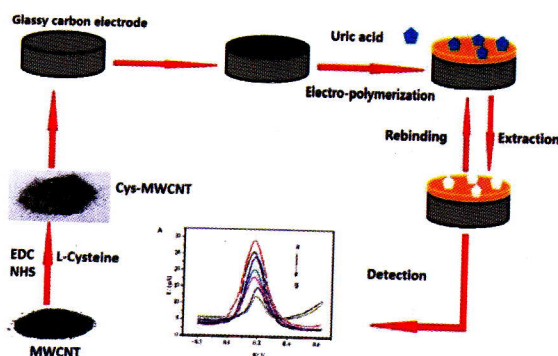
SEPTEMBER 2021

CONTENTS

Papers

- 1151 **Molecularly imprinted electrochemical sensor based on electrode modified by functionalized carbon nanotube for selective detection of uric acid**

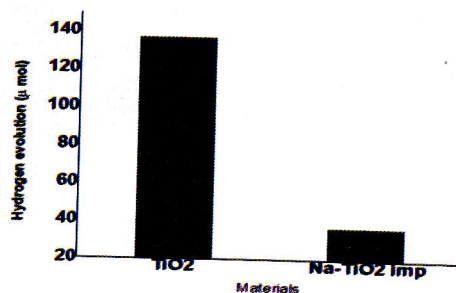
A molecularly imprinted sensor was developed by using electro-polymerization method, with uric acid as the templates, o-diaminobenzene as functional monomers. Using $K_3[Fe(CN)_6]$ as the probe, the imprinted sensor could achieve the detection of uric acid with high selectivity.



Yongfu Zhao*, Hui Liu, Wen Lv & Yanhuan Wang

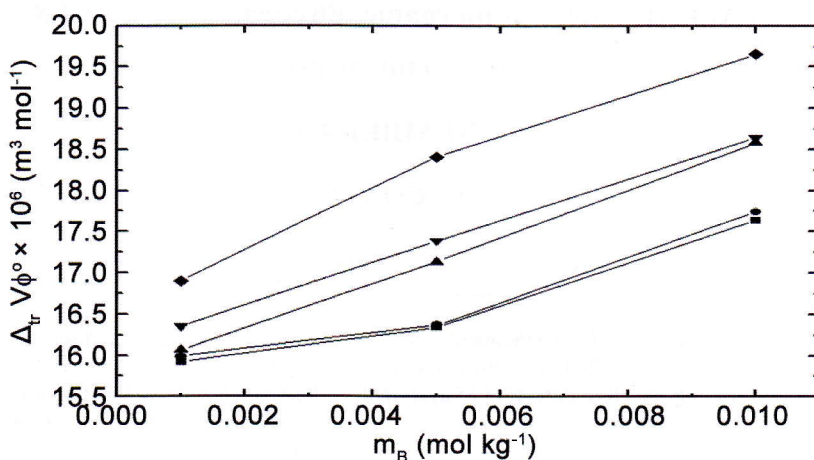
- 1159 **Impact of sodium ion impregnation on the photocatalytic hydrogen evolution activities of anatase/rutile mixed phase TiO_2 nanomaterials**

Sodium ion impregnated anatase/rutile mixed phase TiO_2 material has been synthesised by sol-gel method and characterised for understanding the solar hydrogen production activities. The presence of sodium ion can influence the crystallinity, crystallite size and photocatalytic efficiency of mixed phase TiO_2 .



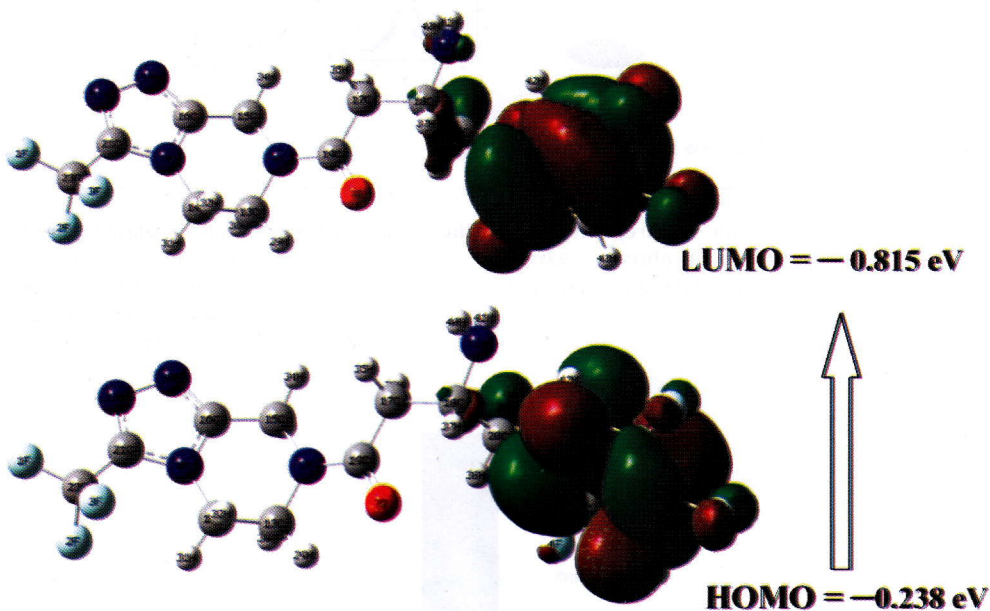
Sruthy Raj P, Prathyusha K R, Resmi M R, Sreenivasan Koliyat Parayil*

- 1164 **Interaction studies of diglycine with aqueous solutions of sulphathiazole drug at different temperatures** Molecular interactions of diglycine in (0.001, 0.005 and 0.010) mol kg⁻¹ aqueous solutions of sulphathiazole drug have been analysed by standard partial molar volume of transfer that has been calculated from density data at (288.15 to 308.15) K under 1.0 MPa pressure.



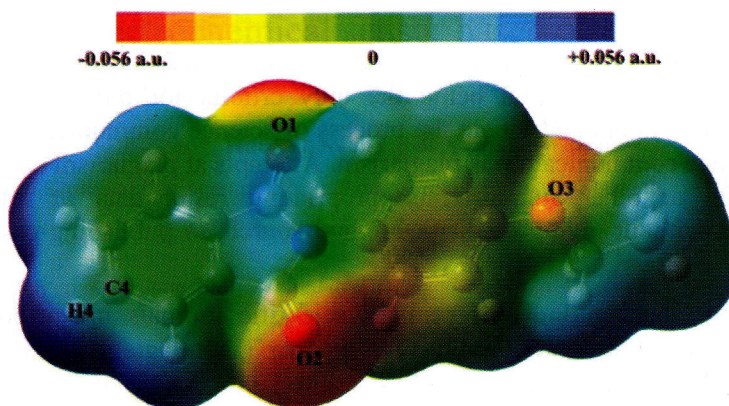
Amalendu Pal* & Surbhi Soni

- 1172 **Spectroscopic characterization and electronic structure analysis of Linagliptin by DFT method** The optimized molecular structure, electronic properties, dipole moment, rotational constants and important thermodynamic parameters of Linagliptin molecule have been computed using Hartree-Fock and density functional theory methods with 6-311++G (d,p) basis set.



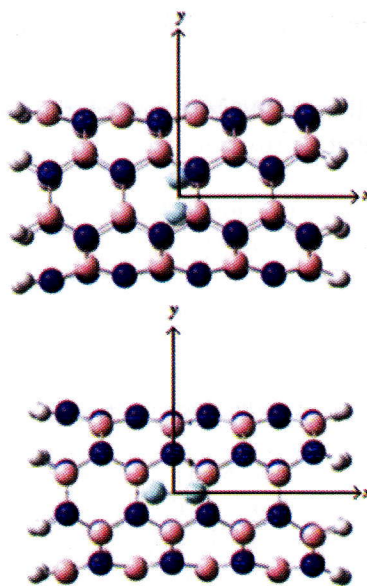
Vijayakumar Balasubramanian*, Sathyanarayanamoorthi Venkatachalam, Kannappan Venu & Naresh Kumar Palanisamy

- 1181 **Molecular structure, spectroscopic and DFT studies of 2-(4-ethoxyphenyl) isoindoline-1,3-dione** Density functional theory calculations of the molecular structure and vibrational spectra have been performed using the B3LYP/6-311++G(d,p) level of theory for 2-(4-ethoxyphenyl)isoindoline-1,3-dione. The theoretical results are compared with the experimental observations.



Meryem Evecen*, Hasan Tanak, Gülcan Duru, Seher Meral & Ayşen Alaman Ağar

- 1192 **Fluorine and chlorine gas storage by confinement inside boron nitrogen nanotubes** DFT calculations were performed to study the interaction between the X_2 ($X=F$ or Cl) molecule and different BNNTs dimensions in parallel or perpendicular position along the nanotube axis.



Yasmine Fatima Zohra Assas, Yamina Belmiloud*, Mohammed Lamine Abdelatif, Soraya Abtouche, Meziane Brahimi & Bahoueddine Tangour

Authors for correspondence are indicated by (*)