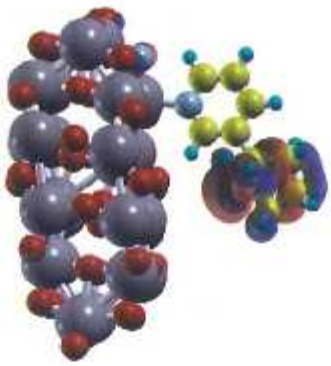
Indian Journal of Chemistry
Sect. A: Inorganic, Bio-inorganic, Physical, Theoretical & Analytical
www.niscair.res.in; http://nopr.niscair.res.in
CODEN: ICACEC; ISSN: 0376-4710 (Print), 0975-0975 (Online)

VOLUME 55A **NUMBER 10** **OCTOBER 2016**

CONTENTS

1182 **Molecular adsorption study of nicotine on the nitrogen doped TiO_2 anatase nanoparticles: Insights from van der Waals corrected DFT computations**

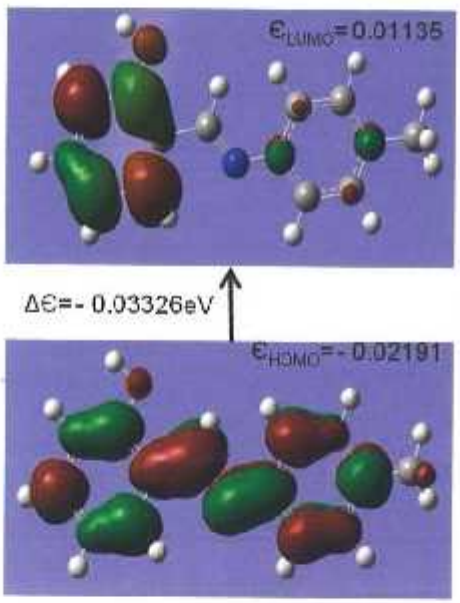
Interaction between nicotine and N-doped TiO_2 nanoparticles is stronger than that between nicotine and pristine TiO_2 nanoparticles. The nitrogen atom of nicotine molecule tends to be strongly adsorbed on the five-fold coordinated titanium site of N-doped anatase nanoparticles. Due to the van der Waals interactions between nicotine molecule and TiO_2, the adsorption on the N-doped TiO_2 is energetically more favorable than that on the pristine one.



Amirali Abbasi* & Jaber Jahanbin Sardroodi

1192 **Experimental and theoretical studies on the structure, electronic and vibrational spectra of *o/p*-hydroxybenzylidene-*o/p*-toluidines**

The theoretical geometry optimization coupled with vibrational and electronic spectral studies of some tailor made aldimines reveal that the two benzene rings of the aldimines are out-of-plane with respect to azomethine linkage. The possible bonding sites of aldimines have been predicted by molecular electrostatic potential analysis.



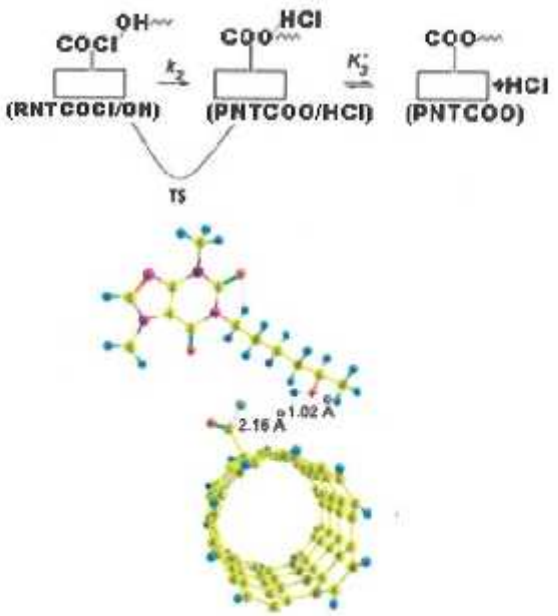
P Suna, P Hota & P K Misra*

Notes

1202 **Quantum mechanical study of carbon nanotubes functionalized with drugs pentoxifylline and lysofylline**

Elham Jalayeri, Ali Morsali* & Mohammad R Bozorgmehr

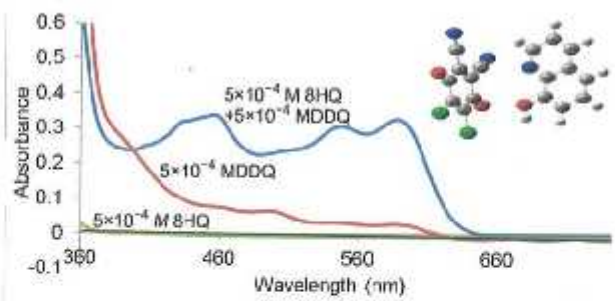
Noncovalent interactions of pentoxifylline with (5, 5) pristine and COOH functionalized-CNTs and the mechanisms of covalent functionalization of lisofylline with (5, 5) COOH and COOCl functionalized CNTs have been studied by DFT calculations. Binding of PTX with COOH functionalized CNT is thermodynamically favorable. COOH and COCl functionalized CNT can bind to lysofylline via OH (COOH mechanism) and Cl (COCl mechanism). The COOH mechanism has higher activation energy than the COCl mechanism, and hence the COCl pathway is suitable for covalent functionalization.



1209 **Charge transfer interaction of 8-hydroxyquinoline with DDQ: Spectrophotometric, thermodynamic and molecular modeling studies**

Baindla Naveen, Lakkadi Arunapriya & Tigulla Parthasarathy*

The absorption spectra of DDQ, 8HQ and their CTC solutions in acetonitrile medium confirms the formation of the charge transfer complex. Multi-charge transfer bands are observed at 456, 548 and 588 nm in the spectra of the CT complex. K_{CT} increases and ε_{CT} decreases as the temperature decreases, which gives an indication of the relative strength of the donor.



Authors for correspondence are indicated by (*)