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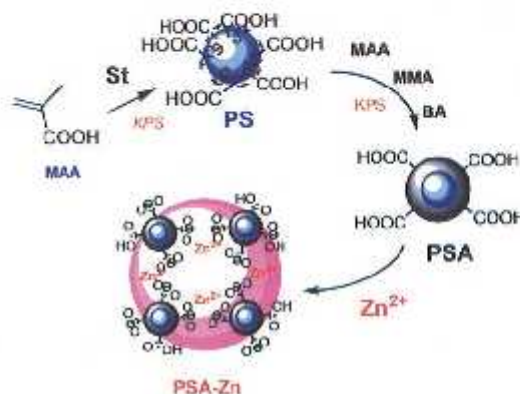
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CONTENTS

1167 Ionically crosslinked core-shell particles for waterborne humidity-sensitive coatings

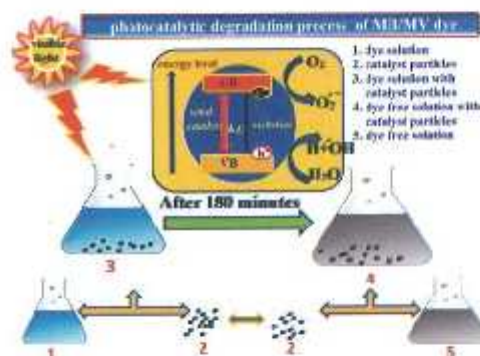
Using zinc ion as ionic crosslinker, a novel self-crosslinked core-shell styrene acrylic ionomer latex (PSA-Zn) has been prepared and characterized. The adhesive force, hardness and thermal stability of PSA-Zn film are better than that of PSA and emulsifier-free acrylate copolymer film coatings. Also, PSA-Zn coating significantly decreases or increases relative humidity in response to environmental humidity in the artificial climate.



Yusheng Wang, Chen Li, Wenzhong Zhai, Yu-Feng He*, Pengfei Song, Yubing Xiong & Rong-Min Wang*

1174 Synthesis, characterization and photocatalytic activity studies of tellurium containing defect pyrochlores, $MSn_{0.5}Te_{1.5}O_6$ ($M = K, Ag, Cu_{0.5}$ and $Sn_{0.5}$)

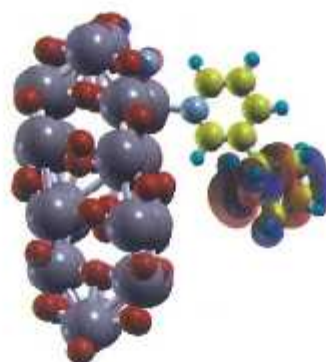
The $AgSn_{0.5}Te_{1.5}O_6$ photocatalyst exhibits higher photocatalytic activity than $MSn_{0.5}Te_{1.5}O_6$ ($M = K, Cu_{0.5}$ and $Sn_{0.5}$) for photodegradation of methylene blue and methyl violet. The higher photocatalytic of $AgSn_{0.5}Te_{1.5}O_6$ is due to its low band gap energy, which endows a very strong photooxidation ability to produce OH^\bullet and $O_2^{\bullet-}$ radicals as active species.



Ravinder Guje, Ravi Gundeboina, Ramaswamy Kadari, Sreenu K, CH. Sudhakar Reddy, M Malathi, Radha Velchuri & Muga Vithal*

1182 **Molecular adsorption study of nicotine on the nitrogen doped TiO₂ anatase nanoparticles: Insights from van der Waals corrected DFT computations**

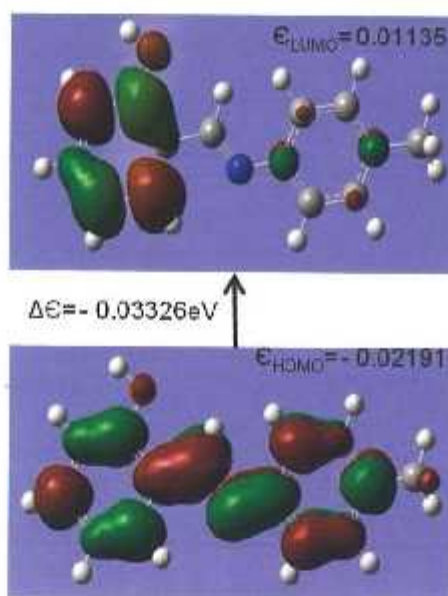
Interaction between nicotine and N-doped TiO₂ nanoparticles is stronger than that between nicotine and pristine TiO₂ nanoparticles. The nitrogen atom of nicotine molecule tends to be strongly adsorbed on the five-fold coordinated titanium site of N-doped anatase nanoparticles. Due to the van der Waals interactions between nicotine molecule and TiO₂, the adsorption on the N-doped TiO₂ 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.

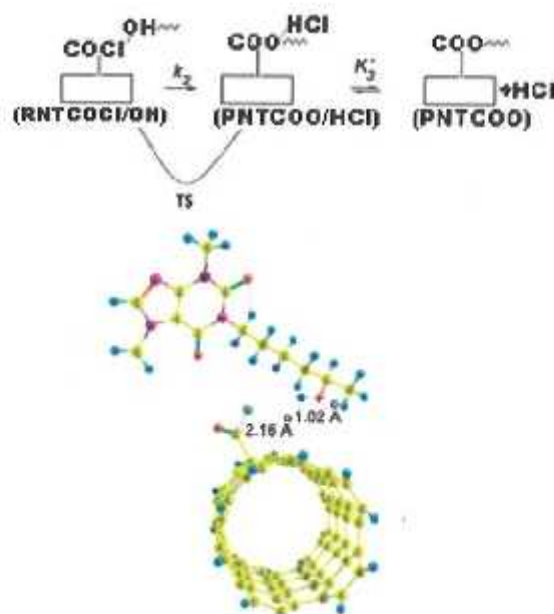


P Suna, P Hota & P K Misra*

Notes

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

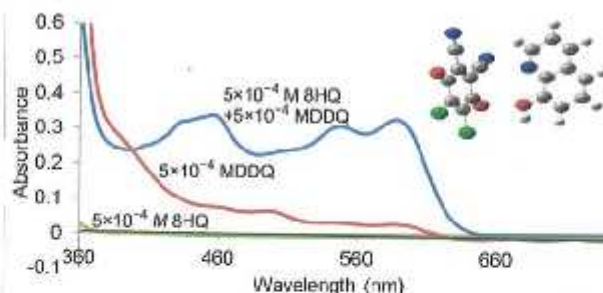
Noncovalent interactions of pentoxifylline with (5, 5) pristine and COOH functionalized-CNTs and the mechanisms of covalent functionalization of lysofylline with (5, 5) COOH and COCl functionalized CNTs have been studied by DFT calculations. Binding of PTX with COOH functionalized CNT is thermodynamically 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.



Elham Jalayeri, Ali Morsali* & Mohammad R Bozorgmehr

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

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.



Baindla Naveen, Lakshmi Arunapriya & Tigulla Parthasarathy*