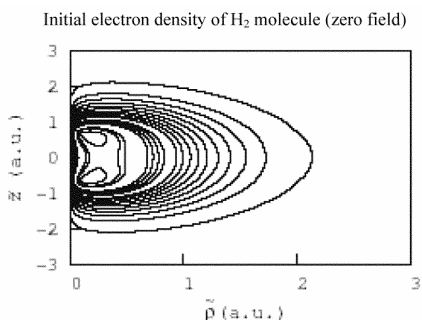


## CONTENTS

### Special issue on Theoretical Chemistry Symposium 2006

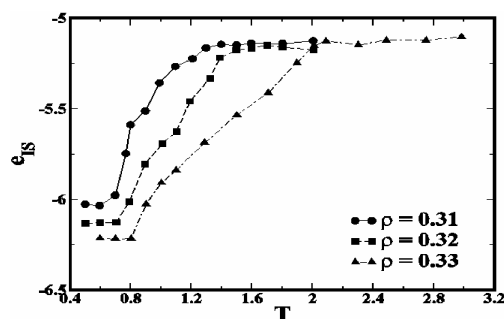
Foreword ..... 333



#### Time-dependent quantum fluid density functional theory of hydrogen molecule under intense laser fields

Amita Wadehra and B M Deb ..... 335–341

Femtosecond dynamics of hydrogen molecule under high intensity laser fields are probed by combining density functional theory and quantum fluid dynamics in three-dimensional space. High harmonics generation and various time-dependent quantities, namely, electron density, ground-state survival probability and dipole moment are studied for different laser wavelengths and intensities.



#### Orientalional dynamics and energy landscape features of thermotropic liquid crystals: An analogy with supercooled liquids

Biman Jana and Biman Bagchi ..... 343–350

Orientalional dynamics and energy landscape features of thermotropic liquid crystals near I–N transition have been compared with features observed for supercooled liquid. The onset of growth of the depth of  $\langle e_{IS} \rangle$  has been correlated with the onset of breakdown of Arrhenius temperature dependence of relaxation time.

$$H_{ret} = \frac{e_1 e_2}{2m_2 c r} [\alpha_1 \times p + \hat{r} \times \alpha_1 \hat{r} \times p]$$

#### Retarded Boson–Fermion interaction in atomic systems

Sambhu N Datta ..... 351–356

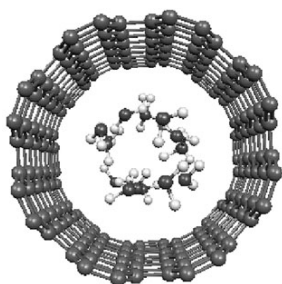
The retarded interaction between an electron and a spin-0 nucleus, derived from electro-dynamical perturbation theory, is discussed here. The retarded form is correct through order  $v^2/c^2$ . Use of the relative coordinates leads to an effective one-electron operator that can be used through all orders of perturbation theory.

$$k_{GL} = \left[ \frac{2\pi}{\hbar^2} \lambda k_B T \right]^{-1/2} \exp \left[ -\frac{(\hbar\omega_0 + \lambda)^2}{2\lambda k_B T} \right] \times I_0 \left( 2\sqrt{S} x \frac{\hbar\omega_0 (\hbar\omega_0 + \lambda)}{\lambda k_B T} \right)$$

#### Quantum electron transfer processes induced by thermo-coherent state

Sumana Banerjee and Gautam Gangopadhyay ..... 357–366

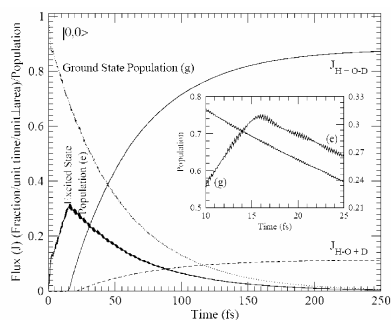
When the reactant surface is not in a thermal equilibrium but in a thermo-coherent state we have derived the rate and discussed about the quantum features of the rate. We have investigated the dependence of temperature on the rate due to displacement, distortion of the harmonic potential energy surfaces of the reactant and product manifold.



### Filled and empty states of carbon nanotubes in water: Dependence on nanotube diameter, wall thickness and dispersion interactions

Malay Rana and Amalendu Chandra ..... 367–376

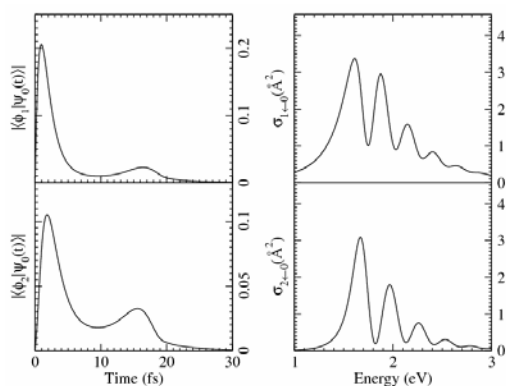
Molecular dynamics simulations of water containing a narrow carbon nanotube as a solute are carried out to investigate the hydration characteristics of the nanotube for different solute-water interaction, system size and also for different diameter and wall thickness of the nanotube.



### Selective control of HOD photodissociation using CW lasers

Manabendra Sarma, S Adhikari and Manoj K Mishra ..... 377–384

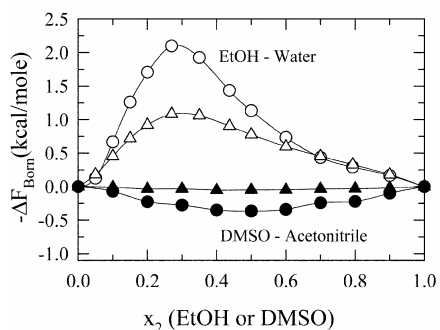
Selective control of HOD photo-dissociation ( $\text{H-O} + \text{D} \leftarrow \text{HOD} \rightarrow \text{H} + \text{O-D}$ ) has been theoretically investigated using CW lasers with appropriate carrier frequency and single vibrational initial state. Results indicate both selectivity and large flux yield (J) in the chosen  $\text{H} + \text{O-D}$  or  $\text{H-O} + \text{D}$  channel may be achieved using simple CW lasers. Further improvements result from the use of Field Optimized Initial State (FOIST) based combination of initial states.



### Calculation of vibrational excitation cross-sections in resonant electron-molecule scattering using the time-dependent wave packet (TDWP) approach with application to the ${}^2\Pi$ $\text{CO}^-$ shape resonance

Raman Kumar Singh, Manabendra Sarma, Ankit Jain, Satrajit Adhikari and Manoj K Mishra ..... 385–389

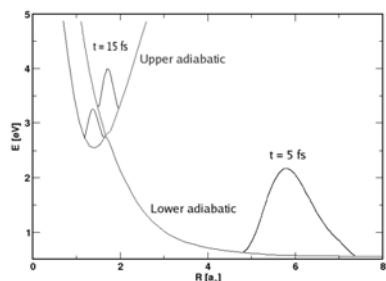
A newly developed time dependent wave packet (TDWP) approach to the calculation of vibrational excitation cross-sections has been applied to formation and decay of the  ${}^2\Pi$   $\text{CO}^-$  shape resonance in e-CO scattering. The results show that the SCF level local complex potential (LCP) in conjunction with the TDWP approach can reproduce experimental features quite satisfactorily.



### Non-ideality in born-free energy of solvation in alcohol-water and dimethylsulfoxide-acetonitrile mixtures: Solvent size ratio and ion size dependence

Hemant K Kashyap and Ranjit Biswas ..... 391–399

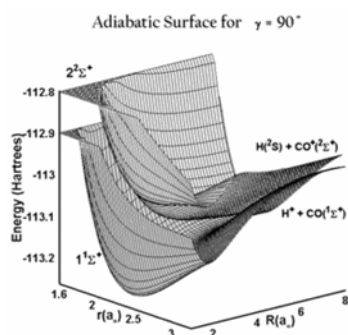
Mean Spherical Approximation (MSA) predicts that non-ideality in Born free energy of solvation of a uni-positive ion in ethanol-water mixture is more pronounced than in dimethylsulfoxide-acetonitrile mixture.



**Reactive chemical dynamics through conical intersections**

S Ghosal, B Jayachander Rao and S Mahapatra ..... 401–407

Nuclear dynamics in terms of quantum wave packet in a nonadiabatic chemical reaction. The wave packet approaches the seam of conical intersections in time (~ 15 fs) and transits to the electronic excited state during the course of reaction taking place on the electronic ground state.



**Diabatic potential energy surfaces of  $H^+ + CO$**

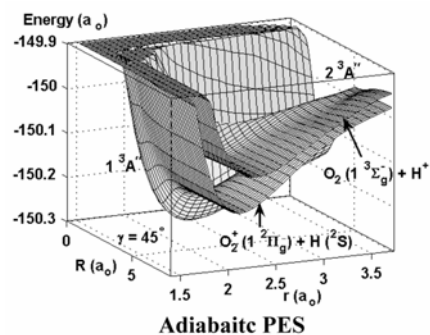
F George D X and Sanjay Kumar ..... 409–415

Completely new and accurate *ab-initio* adiabatic and diabatic potential energy surfaces have been obtained for the  $H^+ + CO$  system at the MRCI/cc-pVTZ level for the collinear and perpendicular approaches of  $H^+$  to provide an understanding of coupling dynamics of inelastic and charge transfer process.

**Effective Floquet Hamiltonian for spin  $I = 1$  in magic angle spinning NMR using contact transformation**

Manoj Kumar Pandey and Mangala Sunder Krishnan ..... 417–422

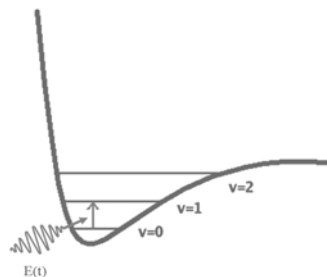
This article presents a theory for the study of first order quadrupolar interactions of a nuclear spin with  $I = 1$  under magic angle spinning conditions in the presence of an external radiofrequency magnetic field. Floquet theory is coupled with van Vleck transformation theory to derive new Floquet Hamiltonians.



**Non-adiabatic collisions in  $H^+ + O_2$  system: An *ab initio* study**

A Saieswari and Sanjay Kumar ..... 423–431

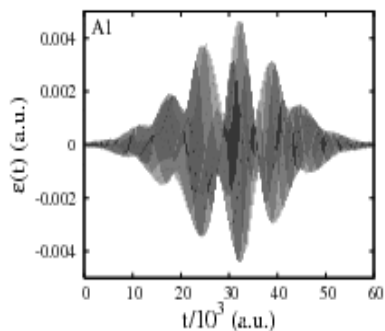
An analysis of the nonadiabatic interactions in the  $H^+ + O_2$  system and the corresponding diabatic potential energy surfaces have been obtained using the MRCI/cc-pVTZ level. The computed vibrational coupling matrix elements for both inelastic and charge transfer processes qualitatively reflect the vibrational excitation patterns observed in the state-to-state beam experiments.



**Quantum control of vibrational excitations in a heteronuclear diatomic molecule**

Sitansh Sharma, Purshotam Sharma and Harjinder Singh . 433–440

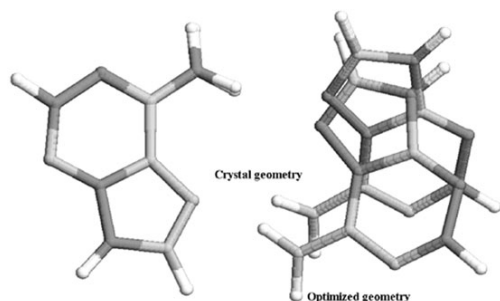
Laser control of vibrational excitations in a heteronuclear diatomic molecule (HF) using Optimal Control Theory. The problem of finding a suitable laser field is phrased in terms of maximization of a cost functional, which is optimized using conjugate gradient method.



### Controlling dynamics in diatomic systems

Praveen Kumar and Harjinder Singh ..... 441–447

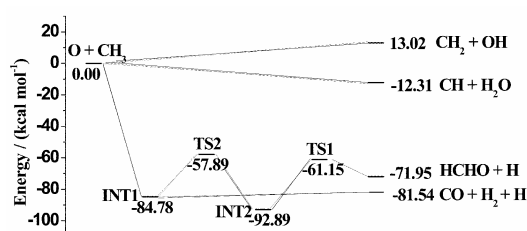
Controlling molecular energetics using laser pulses is formulated for nuclear motion in two different diatomic systems using an iterative method of optimal control. The power spectra of the fields and evolution of populations are obtained.



### Integrated rate expression for the production of glucose equivalent in C<sub>4</sub> green plant and the effect of temperature

Anirban Panda and Sambhu N Datta ..... 449–456

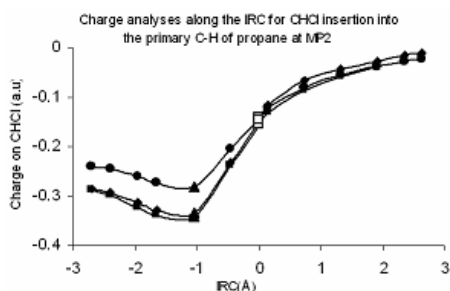
Geometries and interaction energies of noncanonical RNA base pairs in the crystal context and optimized context are examined and compared. These base pairs possess reasonably high interaction energies and slight deformation on optimization indicating inherently stable hydrogen bonding patterns.



### Quantum chemical investigation of the reaction of O(<sup>3</sup>P<sub>2</sub>) with certain hydrocarbon radicals

Ashutosh Gupta, R P Singh, V B Singh, Brijesh Kumar Mishra and N Sathyamurthy ..... 457–465

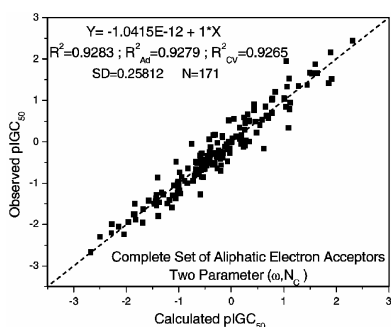
Potential energy profile for the reaction O(<sup>3</sup>P<sub>2</sub>) + CH<sub>3</sub> radical at the CBS-QB3 level of theory.



### Insertion of singlet chlorocarbenes across C–H bonds in alkanes: Evidence for two phase mechanism

M Ramalingam, K Ramasami and P Venuvanalingam ..... 467–473

The singlet chlorocarbenes insertion into C–H bond of methane, ethane, propane and n-butane have been investigated at MP2 and DFT levels using 6–31g(d, p) basis set. The IRC of the TSs have been analysed in terms of Mulliken, NPA and ESP charges to prove the two phase mechanism.



### An atom counting and electrophilicity based QSTR approach

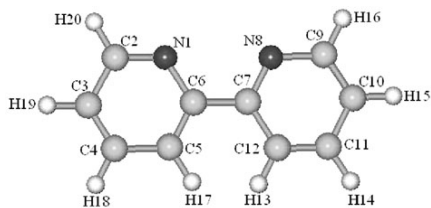
P K Chattaraj, D R Roy, S Giri, S Mukherjee, V Subramanian, R Parthasarathi, P Bultinck and S Van Damme ..... 475–488

A simple descriptor, viz. the number of carbon/non-hydrogenic atoms present in a molecule is prescribed for the development of useful quantitative–structure–toxicity–relationship (QSTR) models which often improve when global/local electrophilicity and/or atomic charges are included as additional descriptors.

### Reactivity descriptors and electron density analysis for ligand chemistry: A case study of 2,2'-bipyridine and its analogues

Bhakti S Kulkarni, Akhilesh Tanwar and Sourav Pal

..... 489–499

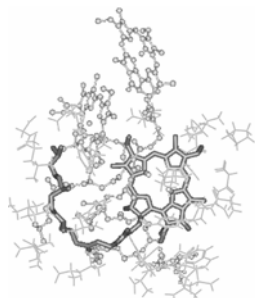


The evaluation of density based local reactivity descriptors using relaxed as well as frozen orbital approximation is discussed for diimines like 2,2'-bipyridine and its analogues.  $\sigma/\pi$  acceptance/donor characteristics of the above ligands is also discussed to explain the formation of supra-molecular assemblies through sigma-pi complexation.

### Theoretical investigation of redox species in condensed phase

Nital Mehta and Sambhu N Datta ..... 501–508

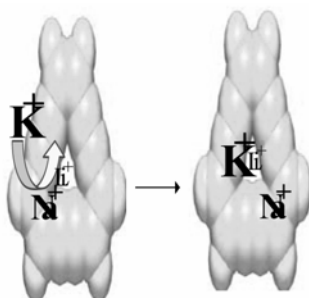
We give a detailed description of the theory and application of explicit as well as implicit solvation treatments for a solute molecule. We especially show how to compute the reduction potential of a biomolecule in a medium. As examples, the reduction potential of Pheophytin-*a* is computed in different environments.



### Metal ion binding with dehydroannulenes – Plausible two-dimensional molecular sieves

B Sateesh, Y Soujanya and G Narahari Sastry ..... 509–515

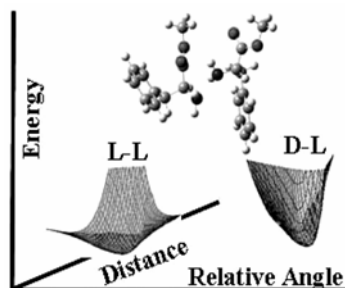
Alkaline earth metal ions bind strongly to dehydroannulenes and the passage through the central cavity is controlled by the size of metal ion and dimension of dehydroannulene cavity.



### Chiral discrimination in biomimetic systems: Phenylalanine

K Thirumoorthy, K Soni, T Arun and N Nandi ..... 517–523

Chiral discrimination is important in peptide biosynthesis. We study the conformational energy variation of methoxy phenylalanine molecule and compared the intermolecular energy surfaces of phenylalanine molecule. The intermolecular energy surface of homochiral pair is more favorable than the corresponding energy surface of heterochiral pair.

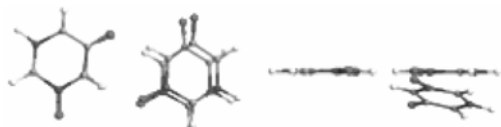


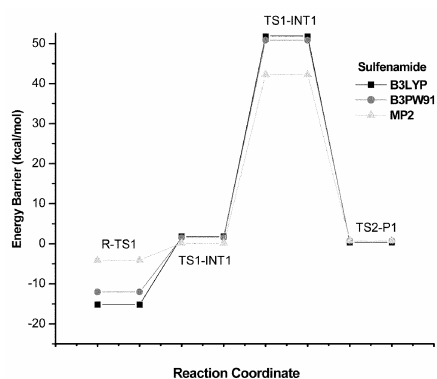
### Base pairing in RNA structures: A computational analysis of structural aspects and interaction energies

Purshotam Sharma, Abhijit Mitra, Sitansh Sharma and

Harjinder Singh ..... 525–531

Geometries and interaction energies of noncanonical RNA base pairs in crystal and optimized contexts are analyzed. Optimization improves planarity of hydrogen bonds by reducing buckle and propeller in base pair geometry. Reasonably high interaction energies and conservation of hydrogen bonding pattern on optimization indicates stability.

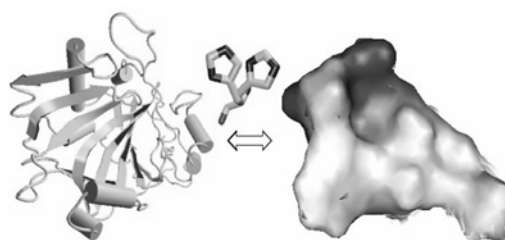




### Reaction mechanism of *O*-acylhydroxamate with cysteine proteases

R Shankar and P Kolandaivel ..... 533–544

The gas-phase reaction mechanism of *O*-acylhydroxamate with cysteine proteases has been investigated using ab initio and density functional theory. On the irreversible process, after breakdown tetrahedral intermediate (INT1), small 1–2 anionotropic has been formed and rearranged to give stable byproducts sulfenamide (P1) and thiocarbamate (P2) with considerable energy loss. While, on the reversible part of this reaction mechanism, intermediate (INT2) breaks down on oxidation, to form a stable product (P3).



### Effect of electrostatic interactions on the formation of proton transfer pathways in human carbonic anhydrase II

Arijit Roy and Srabani Taraphder ..... 545–552

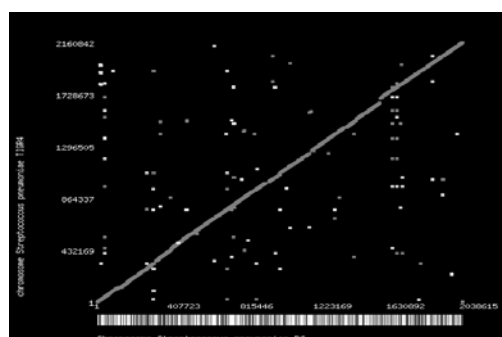
We investigate the role of electrostatic interactions on the formation of dynamical proton pathways through the sidechain conformational fluctuation of His-64 in the enzyme HCA II. The mechanistic implication of our results in the context of shuttling of protons in and out of the active site is also discussed.



### Docking of B-cell epitope antigen to specific hepatitis B antibody

R Rajkannan and E J Padma Malar ..... 553–558

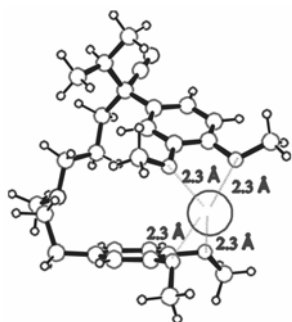
The interaction of pres1 region of hepatitis B virus B-cell epitope antigen with specific hepatitis B neutralizing monoclonal antibody was examined by docking study. The stability of the docked antigen–antibody complex is due to hydrogen bonding and van der Waals interactions.



### On the analysis of the virulence nature of TIGR4 and R6 strains of *Streptococcus pneumoniae* using genome comparison tools

R Jothi, K Manikandakumar, K Ganesan and S Parthasarathy ..... 559–563

Comparative results of genome features, whole genome alignment and gene role category particularly virulence factors between TIGR4 and R6 of *Streptococcus pneumoniae* show the important proteins associated with the strain uniqueness and pathogenesis variations. Low identity between the virulence factors including capsular polysaccharides of R6 with TIGR4 shows the avirulence nature of R6.

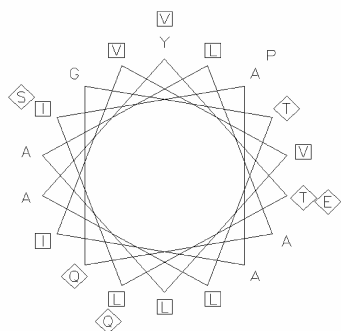


Verapamil ...Ca<sup>2+</sup> (ion holding by drug)

### Phenylalkylamines as calcium channel blockers

Anamika Awasthi and Arpita Yadav ..... 565–570

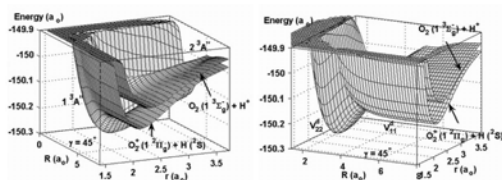
In this study *ab initio* HF coupled with intermolecular interaction calculations have been performed to study mechanistic aspects of benzothiazepines. It is predicted that ternary complex i.e. drug Ca<sup>2+</sup> channel stability may determine potency regulation in these drugs.



### *In silico* characterization of antifreeze proteins using computational tools and servers

K Sivakumar, S Balaji and Gangaradhakrishnan ..... 571–579

Sequence analysis and characterization of seventeen fish antifreeze proteins retrieved from Swiss-Prot database have been done using various computational tools and servers. Identification, visualization and analysis of transmembrane regions and disulphide bonds have also been carried out.



*Cover picture:* Potential energy surfaces for the H<sup>+</sup> + O<sub>2</sub> system; active binding sites in hepatitis B antibody. For details see the article A Saieswari and Sanjay Kumar (pp 423–431) and R Rajkannan and E J Padma Malar (pp 553–558), respectively.