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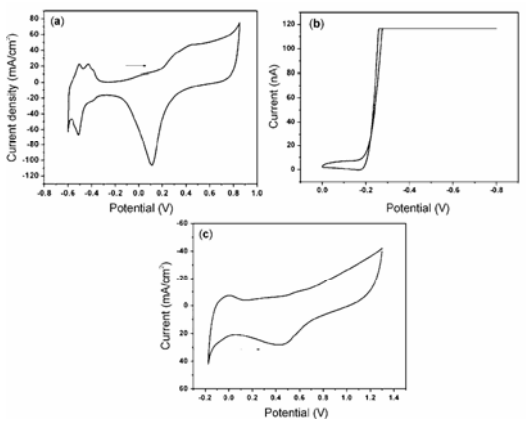
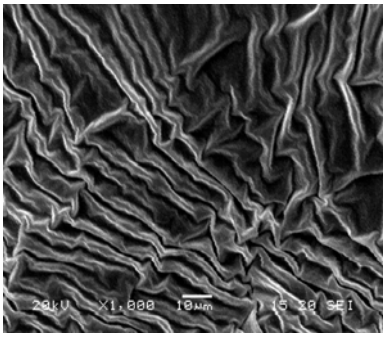
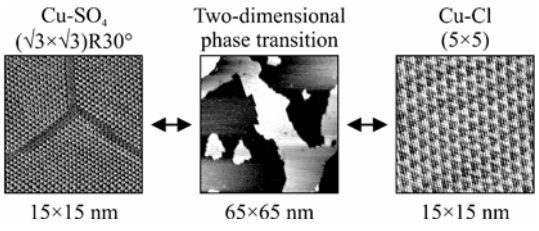
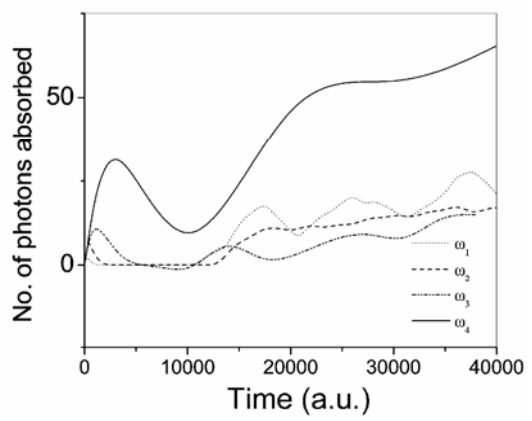
Special issue on Theoretical Chemistry and Electrochemistry







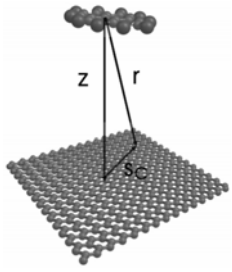


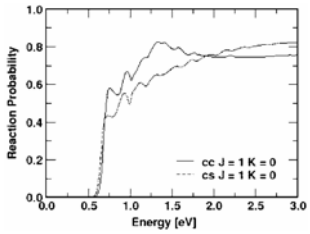
The density operator for a two qubit system with correlated orientations (and polarizations P), for example, is

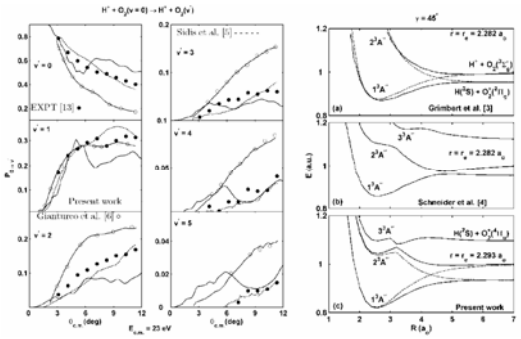
$$\rho^{12} = \frac{1}{4}[(I^1 + P^1.\sigma^1)(I^2 + P^2.\sigma^2) + \sigma^1.\underset{\sim}{C}.\sigma^2]$$

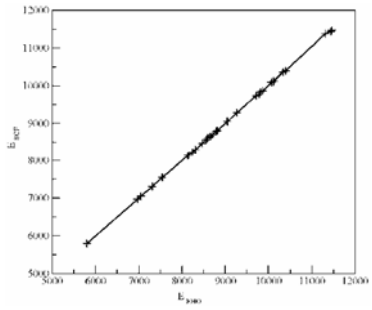
where $\underset{\sim}{C}$ is the correlation tensor with coefficients $(i, j = x, y, z)$

$$C_{ij}^{12} = \langle\sigma_i^1\sigma_j^2\rangle - \langle\sigma_i^1\rangle\langle\sigma_j^2\rangle.$$







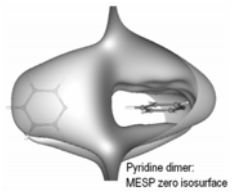


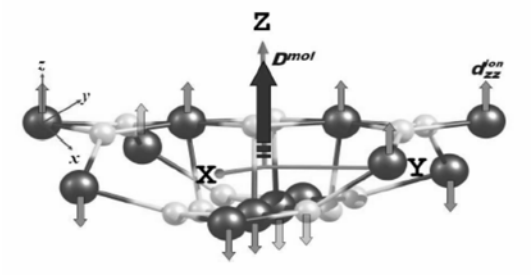
$$L^{\mathrm{T}}FL = \Lambda$$

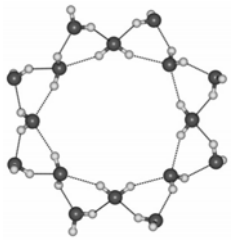
is equivalent to

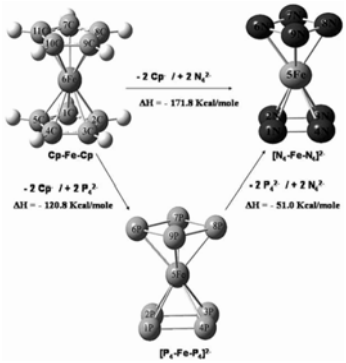
$$\sum_i c_i f_i = \lambda_i$$
$$\sum_j c_j f_j = 0$$

Gaussian elimination gives the relations between f_i.



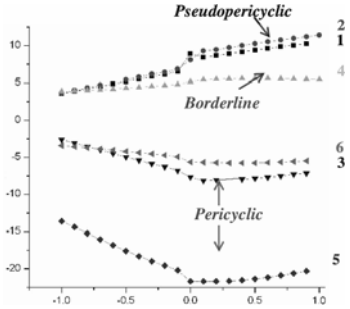






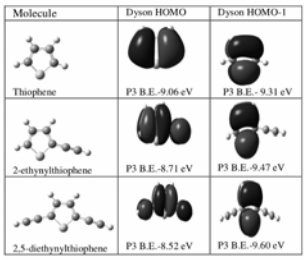
Bonding, aromaticity and reactivity patterns in some all-metal and non-metal clusters

Several sandwich-like metal clusters have been studied at the B3LYP/6-311 + G* level of theory. Bonding and reactivity have been analysed through various geometrical parameters and conceptual density functional theory-based global reactivity descriptors. Aromaticity patterns have been understood in terms of the associated nucleus independent chemical shift values. Possibility of bond-stretch isomerism in some doped clusters is explored. Preferable sites for electrophilic and nucleophilic attacks have been identified using different local reactivity descriptors.



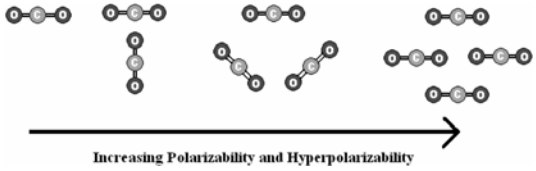
Fluorine effect on pericyclic and pseudopericyclic processes: Evidences and *ab initio* theory

Fluorine substitution increases the pseudopericyclic character of the electrocyclic ring opening reactions of 2-pyranol and pyran through its lone pair participation in the cyclic overlap of orbitals while it does not affect the pseudopericyclic nature of the electrocyclic ring opening reaction of 2-pyrone.



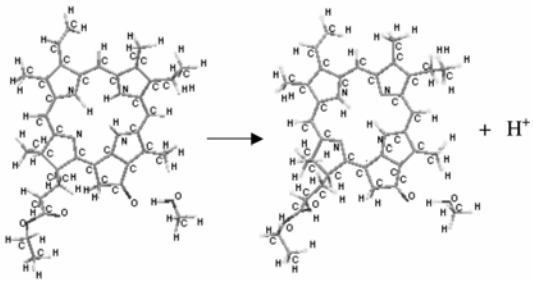
Electronic structure analysis and vertical ionization energies of thiophene and ethynylthiophenes

Dyson orbitals and the corresponding vertical ionization energies for thiophene and ethynylthiophenes have been computed using different decouplings of electron propagator theory. Ring π and ethynyl π_{c-c} electron density distribution of these Dyson orbitals have been analysed for NLO/electrochemical response.



Electronic absorption spectra and nonlinear optical properties of CO_2 molecular aggregates: A quantum chemical study

The quantum chemical calculations of non-linear optical properties of the CO_2 aggregates suggest the application of dense CO_2 in opto-electronic devices.

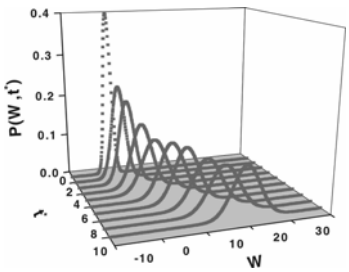


Comparison between implicit and hybrid solvation methods for the determination of pK_a of mono-protonated form of 13^2-(demethoxycarbonyl) pheophytin *a* in methanol

Implicit solvation method (dielectric polarisable continuum model, DPCM) and hybrid solvation method (cluster–continuum model) are adopted to calculate the pK_a of mono-protonated form of 13^2-(demethoxycarbonyl) pheophytin *a* (Pheo) in methanol. The pK_a values of $PheoH^+$ calculated by DFT–DPCM and cluster–continuum methods are 6·12 and 4·70 respectively while the observed value is 4·14. The good performance of the cluster–continuum model over pure continuum model can be attributed to the hydrogen bonding interaction between the solute and the solvent.

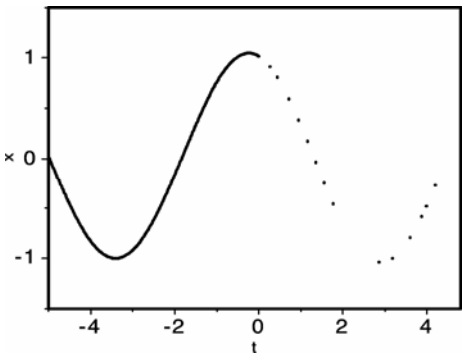
Statistical theory of neutral protein evolution by random site mutations

A self-consistent mean-field theory is developed to evaluate protein neutrality through random single and multiple point mutations by mapping real proteins into a cubic lattice. The results obtained from the theory are in good agreement with the exact enumeration results of the lattice protein and selected real proteins.



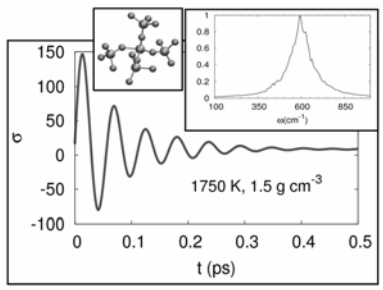
Work distribution for a particle moving in an optical trap and non-Markovian bath

An exact analytical expression of work distribution has been obtained for a system consisting of a colloidal particle trapped in an optical harmonic potential, which is pulled at a constant velocity through a solution represented by a non-Markovian bath composed of an infinite set of harmonic oscillators.



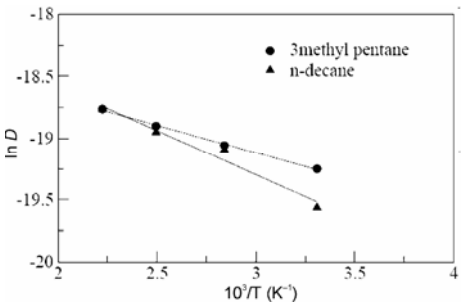
Growth and decay of large fluctuations far from equilibrium

The principle of detailed balance takes care of, on an average, a balance of input of energy into the system through thermal fluctuation and output of energy from the system due to dissipation in a thermally equilibriated system. A 'detailed balance' like condition in the steady state is manifested in the time reversal symmetry between growth and decay of fluctuations far from equilibrium in a non-linear dissipative system characterized by a limit cycle attractor.



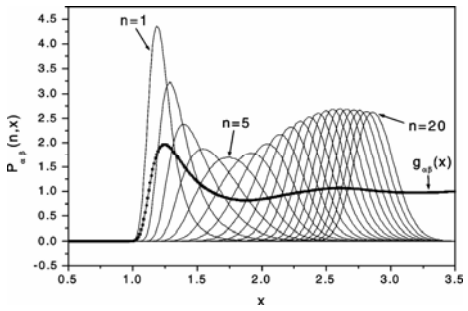
Evaluation of collective transport properties of ionic melts from molecular dynamics simulations

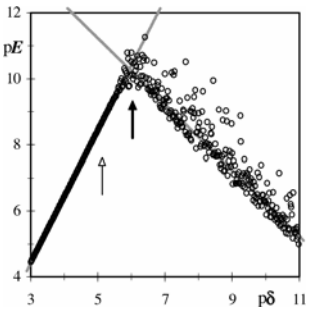
Molecular dynamics simulations of beryllium fluoride have been carried out using a rigid-ion potential model. Transport measures such as the viscosities and ionic conductivities are computed using the Green–Kubo formulation. In addition, structural relaxation times and high-frequency IR-active modes are computed from the pressure and charge-flux auto correlation functions respectively.

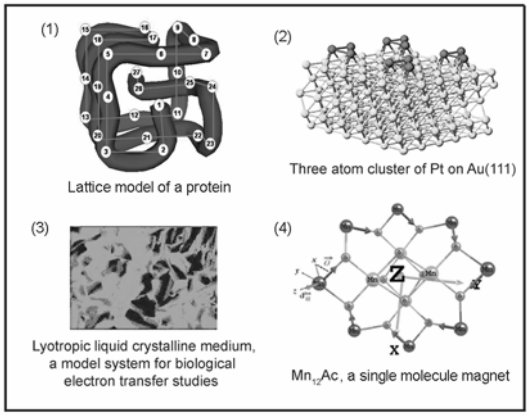


A comparative molecular dynamics study of diffusion of *n*-decane and 3-methyl pentane in Y zeolite

Hydrocarbons in zeolite Y exhibits an anomalous behaviour whereby 3-methyl pentane with larger cross section exhibits a higher diffusivity at low temperatures. This has its origin in the Levitation effect. Lower activation energy for 3-methyl pentane (3·7 kJ/mol) as compared to *n*-decane (6·0 kJ/mol) confirming the origin lies in the Levitation effect.







Cover picture: (1) Lattice model of a protein; for details see the paper by A Bhattacharjee and P Biswas (pp 887–896). (2) Three atom cluster of Pt on Au(111); for details see the paper by E Santos *et al* (pp 575–577). (3) Lyotropic liquid crystalline medium, a model system for biological electron transfer studies; for details see the paper by P Suresh Kumar and V Lakshminarayanan (pp 629–638). (4) $Mn_{12}Ac$, a single molecule magnet; for details see the paper by S Ramasesha *et al* (pp 823–837).

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