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ISSN 1463-9076 CODEN PPCPFQ 11(48) 11349–11672 (2009)



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 Symmetry-breaking plays big  
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*PCCP*, 2009, **11**, 11400.



### Inside cover

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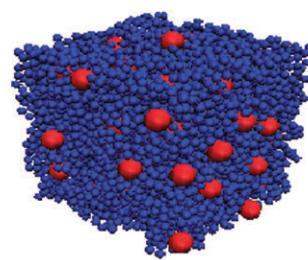
## PERSPECTIVE

11365

### Static, rheological and mechanical properties of polymer nanocomposites studied by computer modeling and simulation

Jun Liu, Liqun Zhang, Dapeng Cao\* and  
 Wenchuan Wang\*

This perspective provides an overview of the progress  
 in the research of polymer nanocomposites by using  
 computer modeling and simulation.



Snapshot of polymer nanocomposites

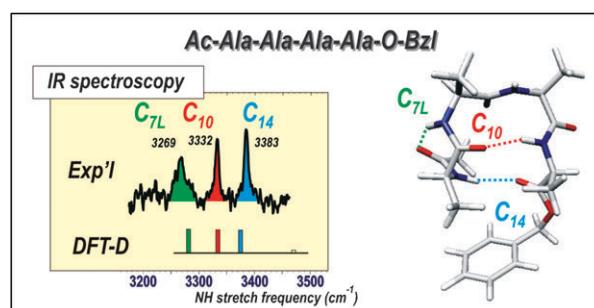
## COMMUNICATIONS

11385

### Gas phase folding of an (Ala)<sub>4</sub> neutral peptide chain: spectroscopic evidence for the formation of a $\beta$ -hairpin H-bonding pattern

Eric Gloaguen, Rodolphe Pollet, François Piuzzi,  
 Benjamin Tardivel and Michel Mons\*

IR and UV laser spectroscopy of an Ala-based 4-residue model peptide recorded under gas phase isolated conditions provides evidence for the intrinsic stability of compact folded structures resembling the extremity of a  $\beta$ -hairpin.



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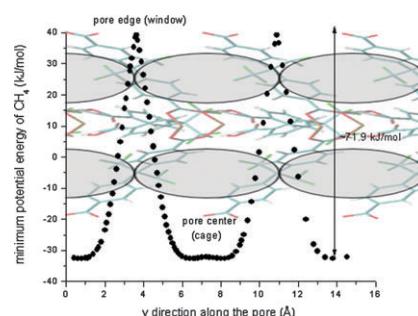
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## COMMUNICATIONS

11389

**Computational identification of a metal organic framework for high selectivity membrane-based  $\text{CO}_2/\text{CH}_4$  separations:  $\text{Cu}(\text{hfipbb})(\text{H}_2\text{hfipbb})_{0.5}$** 

Taku Watanabe, Seda Keskin, Sankar Nair and David S. Sholl\*

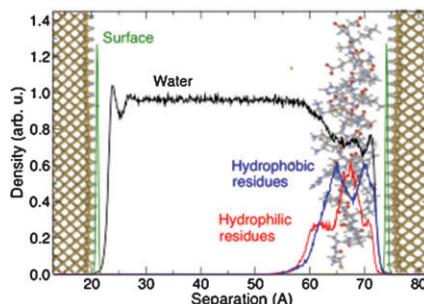
Computational modeling indicates that a small-pore metal organic framework material has unprecedented performance for kinetic separation of  $\text{CH}_4$  and  $\text{CO}_2$ .

11395

**Water structuring and collagen adsorption at hydrophilic and hydrophobic silicon surfaces**

Daniel J. Cole,\* Mike C. Payne and Lucio Colombi Ciacchi

Mutual fit between the hydrophilicity/hydrophobicity pattern and water density oscillations at the solid/liquid interface is demonstrated for collagen adsorbed to H-terminated silicon.

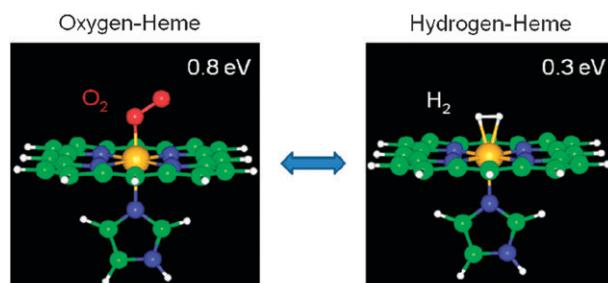


## RESEARCH PAPERS

11400

**Enhanced dihydrogen adsorption in symmetry-lowered metal–porphyrin-containing frameworks**

Yong-Hyun Kim,\* Y. Y. Sun, Woon Ih Choi, Joongoo Kang and S. B. Zhang

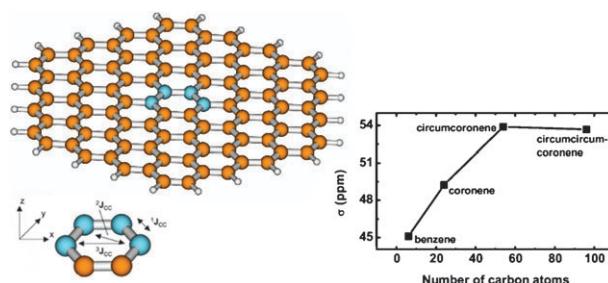
Heme-containing metal–organic frameworks can physisorb molecular hydrogen strongly up to 0.3 eV per  $\text{H}_2$ , as if heme-proteins carry  $\text{O}_2$ .

11404

**NMR tensors in planar hydrocarbons of increasing size**

Suvi Ikäläinen, Perttu Lantto, Pekka Manninen and Juha Vaara\*

Novel basis sets allow quantitative prediction of the anisotropic NMR parameters of planar hydrocarbons at the large-system limit.



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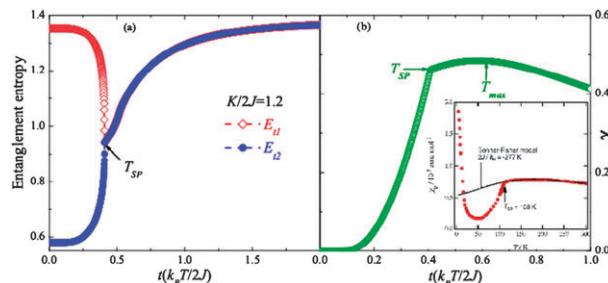
## RESEARCH PAPERS

11415

**Spin-Peierls transition in low-dimensional quantum spin systems: a Green's function approach**

L. J. Ding, K. L. Yao\* and H. H. Fu

The spin-Peierls transition can be detected by the thermal entanglement entropy and magnetic susceptibility, which coincides with the experimental results.

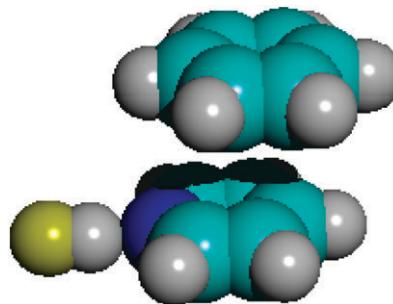


11424

**Cooperativity of  $\pi$ -stacking and hydrogen bonding interactions and substituent effects on X-ben||pyr $\cdots$ H-F complexes**

Ali Ebrahimi, Mostafa Habibi, Razieh Sadat Neyband and Ali Reza Gholipour

Cooperativity arising from interplay of H-bonding and  $\pi$ -stacking interactions might play a role in X-benzene||pyridine $\cdots$ HF complexes.

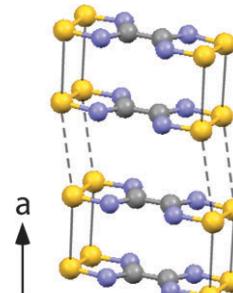


11432

**Electronic structure of disjoint diradical 4,4'-bis(1,2,3,5-dithiadiazolyl) thin films**

Kaname Kanai,\* Hiroyuki Yoshida, Yukiko Noda, Akito Iwasaki, Rie Suizu, Jun'ya Tsutumi, Hiroki Imabayashi, Yukio Ouchi, Naoki Sato, Kazuhiko Seki and Kunio Awaga

Direct observation of the evolution of the  $\pi$ -orbital overlap between the stacked BDTDA dimers into a quasi one-dimensional energy band.

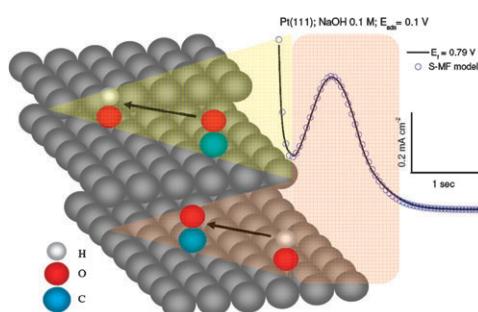


11437

**Mechanism of electro-oxidation of carbon monoxide on stepped platinum electrodes in alkaline media: a chronoamperometric and kinetic modeling study**

Gonzalo García and Marc T. M. Koper\*

Based on transient measurements and modeling, a detailed picture is derived for the oxidation of carbon monoxide on a platinum electrode in alkaline media, highlighting the difference between steps and terrace sites.

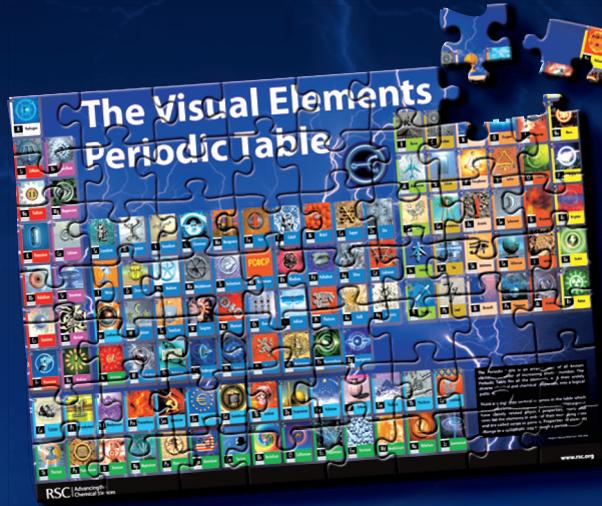
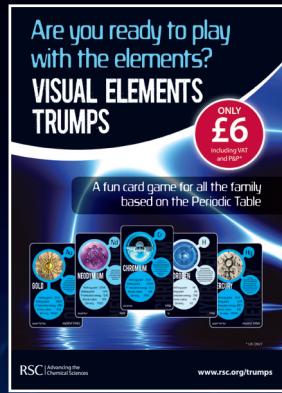


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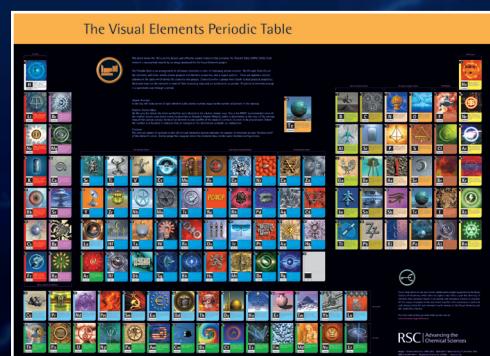
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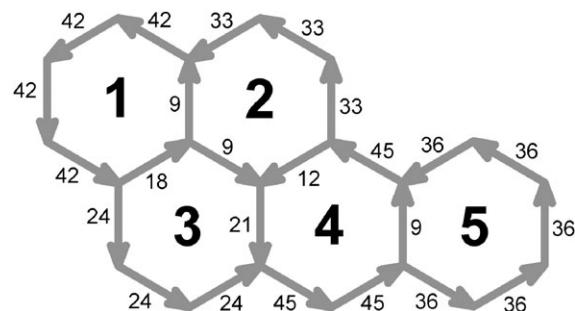


11447

**Graph-topological approach to magnetic properties of benzenoid hydrocarbons**

Arkadiusz Ciesielski,\* Tadeusz M. Krygowski, Michał K. Cyrański, Michał A. Dobrowolski and Jun-ichi Aihara

An effective approach interpreting ring current formation in benzenoid hydrocarbons exposed to an external magnetic field is presented.

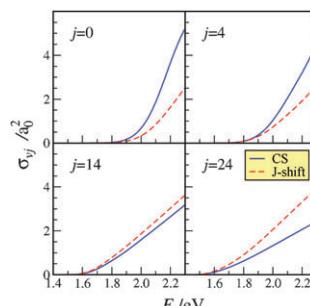


11456

**A detailed comparison of centrifugal sudden and J-shift estimates of the reactive properties of the N + N<sub>2</sub> reaction**

Ernesto García, Carlos Sánchez, Amaia Saracibar, Antonio Laganà and Dimitris Skouteris

J-shift excitation function depends on the initial diatomic rotational energy more weakly than the centrifugal sudden one.

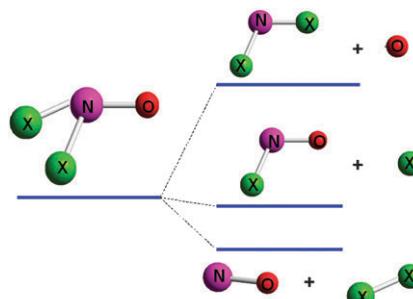


11463

**On the stability of X<sub>2</sub>NO radicals (X = F, Cl, Br, I)**

Cristina Puzzarini and Vincenzo Barone

Stability of X<sub>2</sub>NO radicals (X = F, Cl, Br, I): effects of electron correlation treatment, basis set, core correlation and structure on dissociation energies.

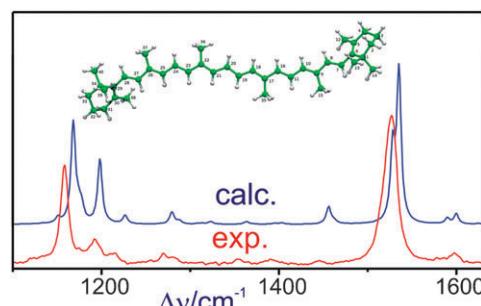


11471

**Resonance Raman spectra of β-carotene in solution and in photosystems revisited: an experimental and theoretical study**

Norman Tscherner, Matthias Schenderlein, Katharina Brose, Eberhard Schlodder, Maria Andrea Mroginski, Christian Thomsen and Peter Hildebrandt\*

Resonance Raman spectroscopy and density functional theory calculations are employed to analyse the excitation-dependent variation of the C=C stretching of β-carotene in photosystems.



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University of Cambridge, UK
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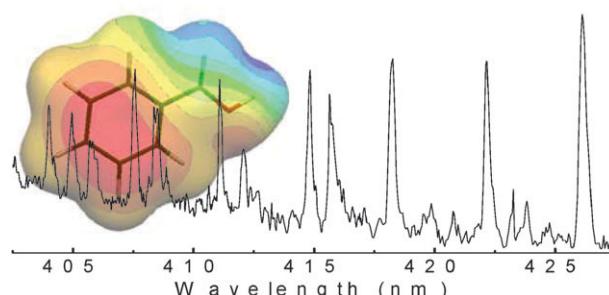


11479

### Electronically excited states of protonated aromatic molecules: benzaldehyde

I. Alata, R. Omidyan, C. Dedonder-Lardeux,\* M. Broquier and C. Jouvet

Protonated benzaldehyde presents a first singlet electronic transition of  $\pi\pi^*$  character in the visible, with well resolved vibrational bands.

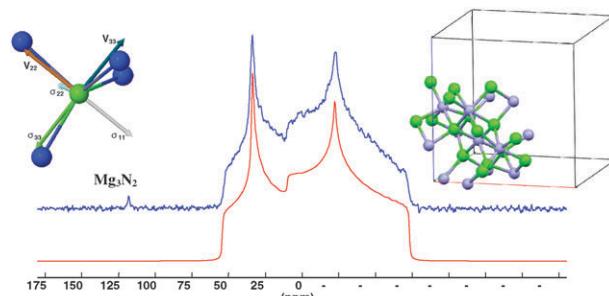


11487

### Mg-25 ultra-high field solid state NMR spectroscopy and first principles calculations of magnesium compounds

Peter J. Pallister, Igor L. Moudrakovski\* and John A. Ripmeester

A combination of 21T  $^{25}\text{Mg}$  solid-state NMR and first principle calculations are employed to reveal structural details of magnesium compounds.

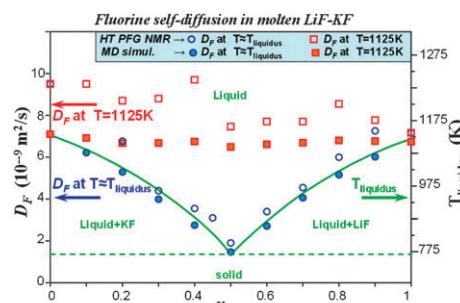


11501

### Diffusion coefficients and local structure in basic molten fluorides: *in situ* NMR measurements and molecular dynamics simulations

Vincent Sarou-Kanian, Anne-Laure Rollet,\* Mathieu Salanne, Christian Simon, Catherine Bessada and Paul A. Madden

Self-diffusion of ions  $D$  in the molten salt LiF–KF varies with the liquidus temperature of the phase diagram.  $D$  is governed weakly by the LiF molar fraction  $x_{\text{LiF}}$  but mostly by temperature. The activation energy is related to the fluoroacidity of the molten salt.

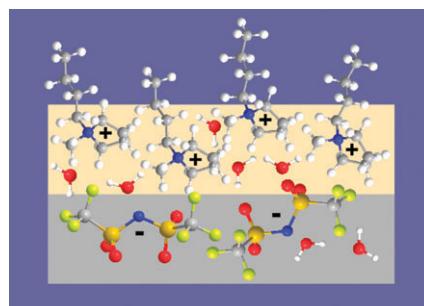


11507

### X-Ray reflectometry studies on the effect of water on the surface structure of $[\text{C}_4\text{mpyr}][\text{NTf}_2]$ ionic liquid

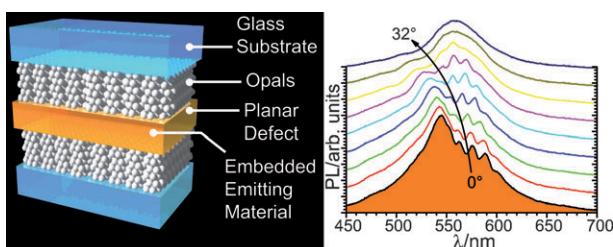
Y. Lauw,\* M. D. Horne, T. Rodopoulos, N. A. S. Webster, B. Minofar and A. Nelson

The structure of an ionic liquid–water mixture at a gas–liquid surface is probed by XRR.



## RESEARCH PAPERS

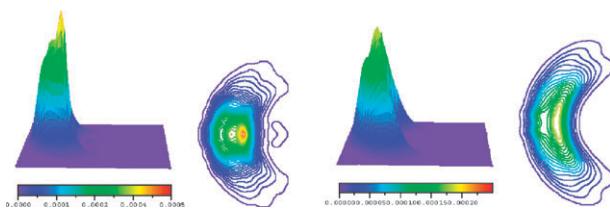
11515

**Amplified spontaneous emission from opal photonic crystals engineered with structural defects**

Francesco Di Stasio, Luca Berti, Martin Burger, Franco Marabelli, Samuele Gardin, Tiziano Dainese, Raffaella Signorini, Renato Bozio and Davide Comoretto\*

We report on the optical properties and amplified spontaneous emissions (ASE) of polystyrene opals engineered with planar structural defects containing a conjugated polymer emitter.

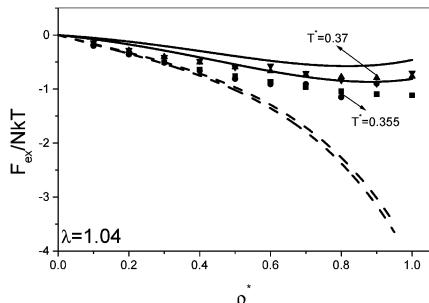
11520

**The OH + D<sub>2</sub> → HOD + D angle-velocity distribution: quasi-classical trajectory calculations on the YZCL2 and WSLFH potential energy surfaces and comparison with experiments at E<sub>T</sub> = 0.28 eV**

José Daniel Sierra, Rodrigo Martínez, Jordi Hernando and Miguel González\*

Comparison of experiments with QCT calculations for OH + D<sub>2</sub> shows that challenges remain for the theory to describe angle-velocity distributions.

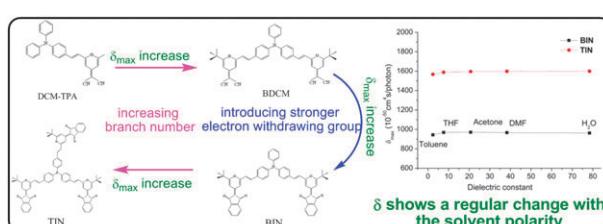
11528

**Low temperature behavior of thermodynamic perturbation theory**

Shiqi Zhou\* and J. R. Solana

$\frac{F_{ex}}{NKT} - \rho^*$  for hard sphere square well fluid. Dashed lines and solid lines are for BH-LCA and 3rd-TPT, respectively.

11538

**Theoretical study of solvent effect on one- and two-photon absorption properties of starburst DCM derivatives**

Yang Zhao, Ai-Min Ren,\* Ji-Kang Feng, Xin Zhou, Xi-Cheng Ai and Wen-Jie Su

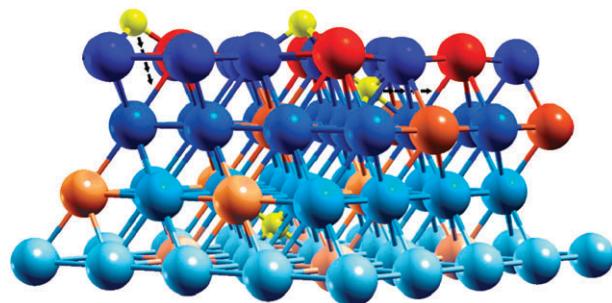
TPA cross section of DCM derivatives shows a regular change with the molecular structure and the solvent polarity.

## RESEARCH PAPERS

11546

**A DFT comparative study of carbon adsorption and diffusion on the surface and subsurface of Ni and Ni<sub>3</sub>Pd alloy**

F. Cinquini, F. Delbecq and P. Sautet\*

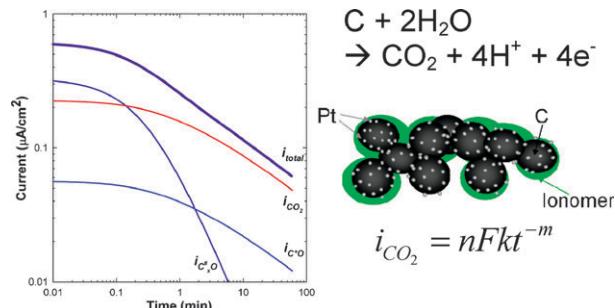
Carbon diffusion processes in Ni<sub>3</sub>Pd compared to Ni, as a key step for carbon nanotubes growth.

11557

**Kinetic model of the electrochemical oxidation of graphitic carbon in acidic environments**

Kevin G. Gallagher\* and Thomas F. Fuller

A mechanism is proposed to explain the complex behavior of the electrochemical oxidation of carbon in aqueous, acidic electrolytes, such as in PEM fuel cells.

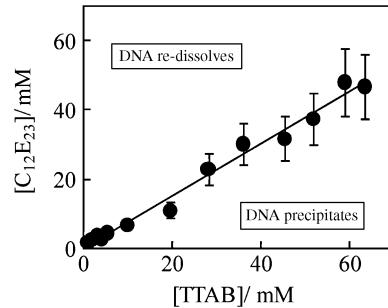


11568

**Re-dissolution and de-compaction of DNA–cationic surfactant complexes using non-ionic surfactants**

Conrad P. Corbyn, Paul D. I. Fletcher,\* Rabia Gemici, Rita S. Dias and Maria G. Miguel

Compacted, water-insoluble complexes of DNA with cationic surfactants can be re-dissolved and de-compacted by addition of non-ionic surfactants at surfactant mixture compositions which are successfully modeled using mixed micelle theory.

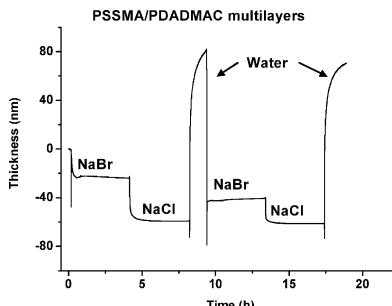


11577

**Influence of salt on assembly and compression of PDADMAC/PSSMA polyelectrolyte multilayers**

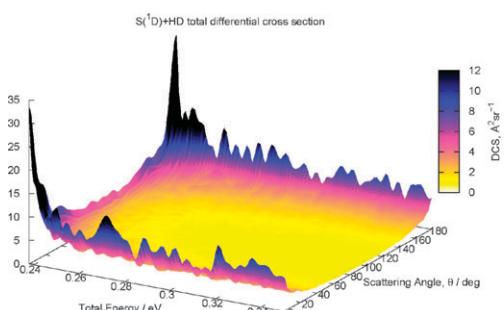
Xiao Gong and Changyou Gao\*

Reversibility of multilayer compression and mechanical properties is mediated by salt incubation.



## RESEARCH PAPERS

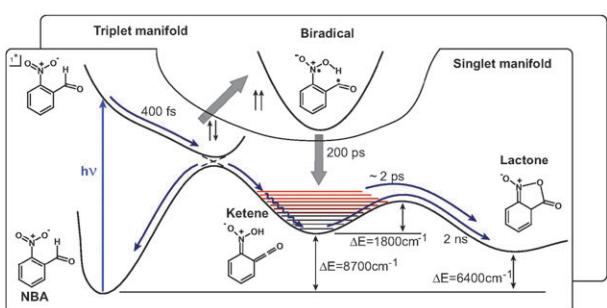
11587

**Integral and differential cross sections for the  $S(^1D) + HD$  reaction employing the ground adiabatic electronic state**

H. Yang, K.-L. Han, G. C. Schatz, S.-H. Lee, K. Liu, S. C. Smith and M. Hankel\*

Fully converged differential cross sections have been calculated for the  $S(^1D) + HD$  reaction for a range of total energies in eV.

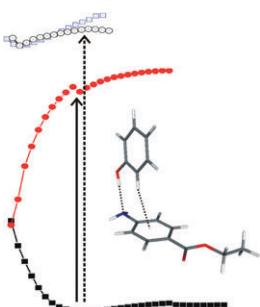
11596

**Impact of vibrational excitation on the kinetics of a nascent ketene**

Thomas Schmierer, Wolfgang J. Schreier, Florian O. Koller, Tobias E. Schrader and Peter Gilch\*

Vibrational excitation of a reactive ground state intermediate results in biphasic kinetics with rate constants differing by several orders of magnitude.

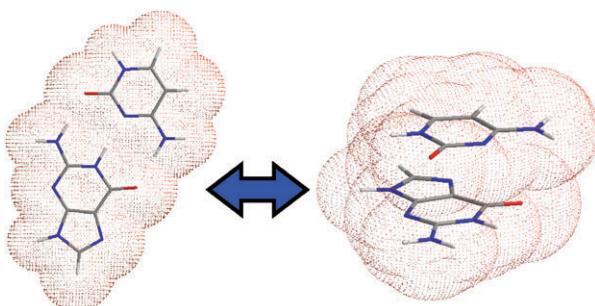
11608

**Molecular recognition in the gas phase: benzocaine–phenol as a model of anaesthetic–receptor interaction**

Edurne Aguado, Iker León, Emilio J. Coccinero, Alberto Lesarri, José A. Fernández\* and Fernando Castaño

Benzocaine–phenol interaction is analyzed in jets as a model of the interaction in the benzocaine receptor.

11617

**Non covalent interactions in RNA and DNA base pairs: a quantum-mechanical study of the coupling between solvent and electronic density**

Filippo Lipparini, Giovanni Scalmani and Benedetta Mennucci\*

A quantum mechanical analysis of the role played by the coupling between correlated electronic densities and solvent polarization in determining the relative importance of hydrogen bonding and stacking in solvated base pairs.

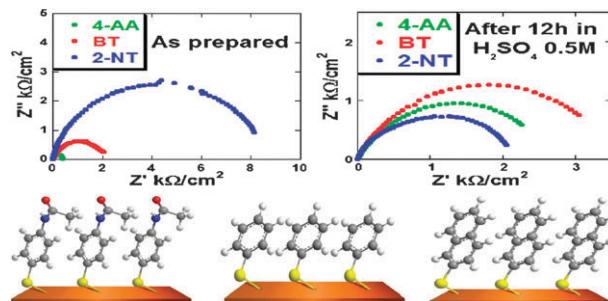
## RESEARCH PAPERS

11624

**A multi-technique approach to the analysis of SAMs of aromatic thiols on copper**

Fabrizio Caprioli,\* Marco Beccari, Andrea Martinelli, Valeria Di Castro and Franco Decker

Different molecular structures of aromatic thiol adlayers are responsible for the Cu passivation behaviour in acidic solution.

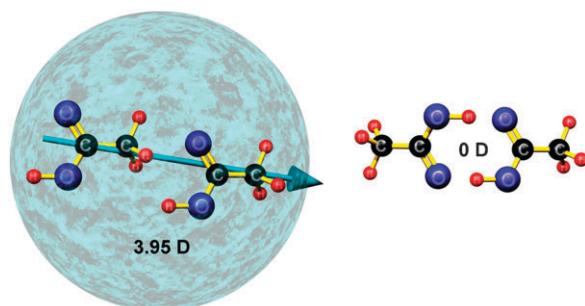


11631

**Electron attachment and electron ionization of acetic acid clusters embedded in helium nanodroplets**

F. Ferreira da Silva, S. Jaksch, G. Martins, H. M. Dang, M. Dampc, S. Denifl, T. D. Märk, P. Limão-Vieira, J. Liu, S. Yang, A. M. Ellis and P. Scheier\*

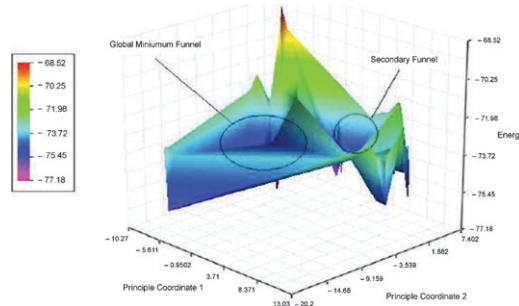
In the low-temperature environment of He droplets acetic acid forms acyclic (head-to-tail) clusters, which have favourable electronic properties for binding helium atoms.



11638

**Principal component analysis of potential energy surfaces of large clusters: allowing the practical calculation of the master equation**

Nima Shariat Panahi and R. S. Berry\*

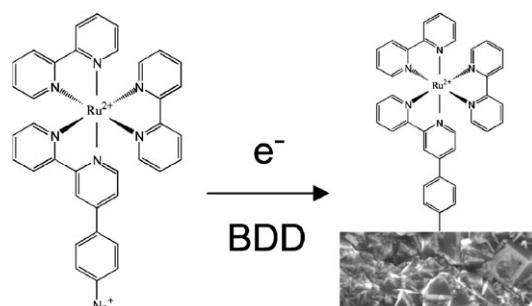
A view of the potential surface of Ar<sub>20</sub>, expressed as a function of the two most important principal coordinates.

11647

**XPS study of ruthenium tris-bipyridine electrografted from diazonium salt derivative on microcrystalline boron doped diamond**

Charles Agnès, Jean-Charles Arnault,\* Franck Omnes, Bruno Jousselme, Martial Billon, Gérard Bidan and Pascal Mailley\*

Boron doped diamond is functionalized by a ruthenium complex film using diazonium salts and characterized by electrochemistry and XPS.



## ADDITIONS &amp; CORRECTIONS

11655

## Additions and corrections published in 2009

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