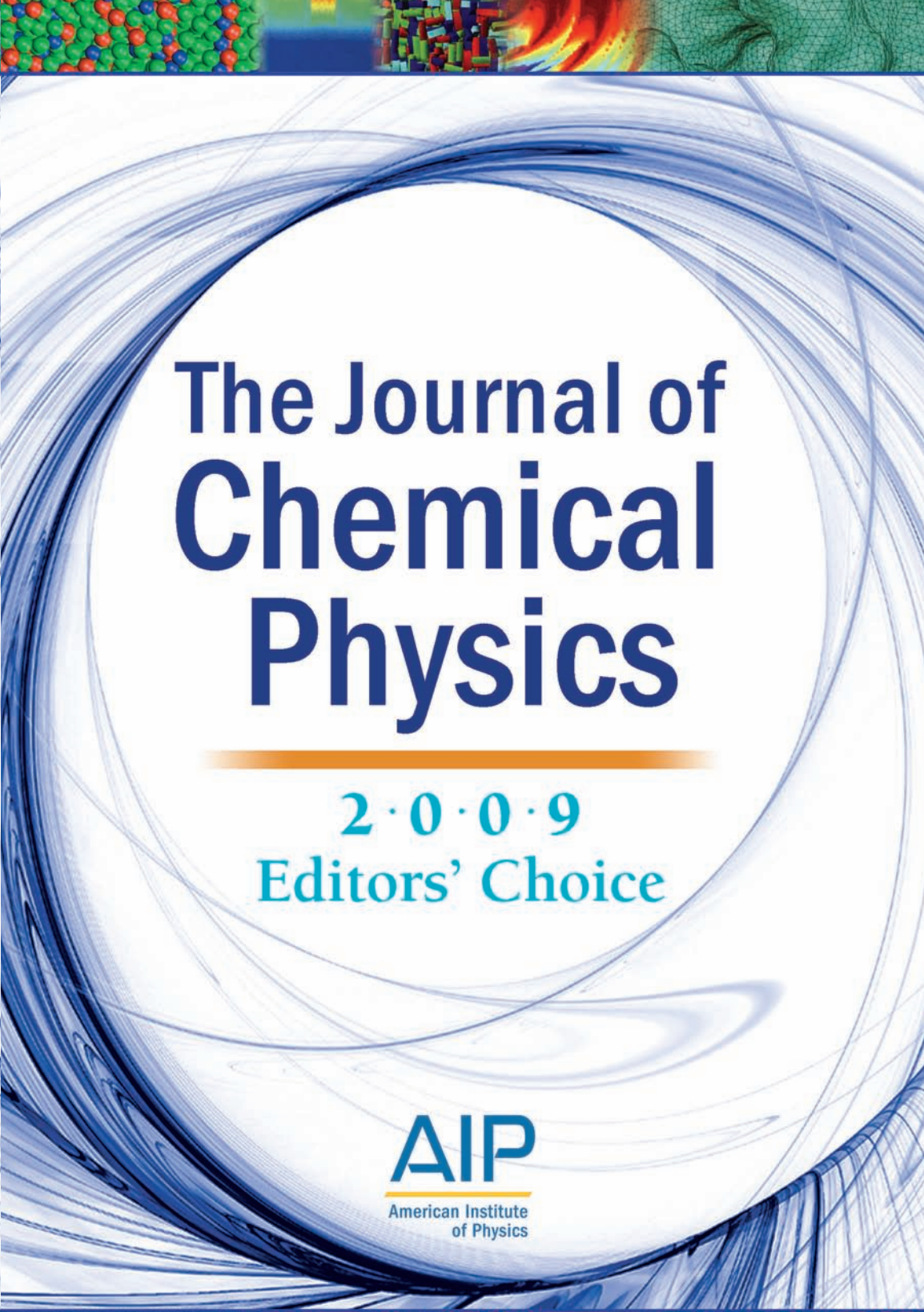

The Journal of
Chemical
Physics
2·0·0·9
Editors' Choice
AIP
American Institute
of Physics
jcp.aip.org/jcp/editors_choices_2009

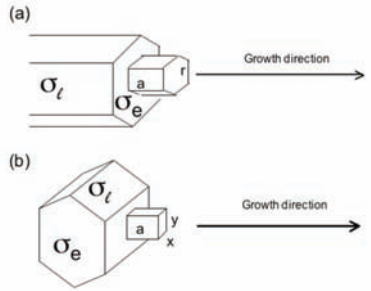
The Journal of Chemical Physics

2009 Editors' Choice

The Editors at *The Journal of Chemical Physics* facilitate publication of the most innovative and influential articles in the field of Chemical Physics each year. In the following collection, the Editors have selected a few of the many notable JCP articles published in 2009 that present ground-breaking research. This collection represents only a small fraction of the critical research published in JCP in 2009 and is representative of the broad cross-section of topics that the journal covers. These seminal articles are freely available online at jcp.aip.org until the end of August 2010.

Theory of competitive adsorption-nucleation in polypeptide-mediated biomineralization

M. Muthukumar



This work deals with the mechanism of biomineralization: the nucleation and growth of mineral structures through interaction with biomolecules. In addressing how specific biopolymers direct selection of mineral morphologies and their growth kinetics, the author presents a new model based on a competition between adsorption of polymers onto selective interfaces and nucleation growth of minerals.

J. Chem. Phys. **130**, 161101 (2009)

$$W(\tau) = \int_{t=0}^{t=\tau} f(t)d\{z[x(t)]\}$$

The work-Hamiltonian connection and the usefulness of the Jarzynski equality for free energy calculations

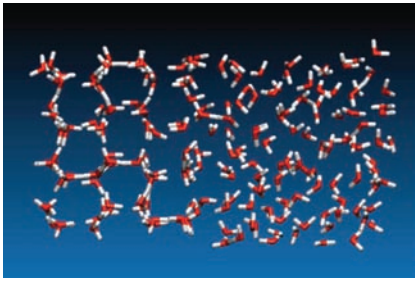
Eric N. Zimanyi and **Robert J. Silbey**

The authors discuss the relationship between two possible definitions of free energy and show how some recent disagreements regarding the applicability of the Jarzynski equality are the result of different authors using different definitions of free energy.

J. Chem. Phys. **130**, 171102 (2009)

On the phase diagram of water with density functional theory potentials: The melting temperature of ice I_h with the Perdew–Burke–Ernzerhof and Becke–Lee–Yang–Parr functionals

Soohaeng Yoo, Xiao Cheng Zeng, and **Sotiris S. Xantheas**



The authors used Born-Oppenheimer molecular dynamics simulation and two commonly used density functionals to investigate the properties of water. They found that ambient condition simulations at $\rho = 1$ g/cm^3 will describe a supercooled state that is overstructured when compared to liquid water.

J. Chem. Phys. **130**, 221102 (2009)

Approaching the Hartree–Fock limit by perturbative methods

Jia Deng, Andrew T. B. Gilbert, and **Peter M. W. Gill**

$$\mathbf{F} = \mathbf{h} + \sum_{j}^{m} (2\mathbf{J}_j - \mathbf{K}_j),$$

Described are perturbative methods for improving finite-basis Hartree–Fock calculations toward the complete-basis limit. The best method appears to offer quadratic error reduction and preliminary numerical applications that demonstrate remarkably accurate Hartree–Fock energies can be obtained.

J. Chem. Phys. **130**, 231101 (2009)

$$\Delta R_{ab}^{ij} \approx \bar{W}_{ab}^{ij} - \sum_{m,n} \langle ab|r_{12}^{-1}|mn\rangle \bar{F}_{mn}^{ij} - \sum_{m,c} [\langle ab|r_{12}^{-1}|mc\rangle \bar{F}_{mc}^{ij} + \langle ab|r_{12}^{-1}|cm\rangle \bar{F}_{cm}^{ij}] - \sum_{c,d\in[ij]} \langle ab|r_{12}^{-1}|cd\rangle \bar{F}_{cd}^{ij} \text{ for } a,b \in [ij],$$

Local explicitly correlated coupled-cluster methods: Efficient removal of the basis set incompleteness and domain errors

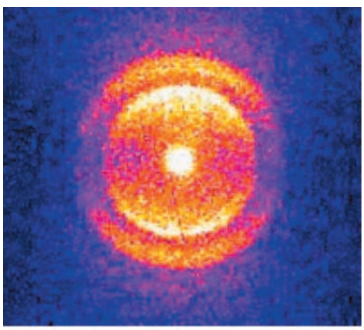
Thomas B. Adler and **Hans-Joachim Werner**

Proposed is an explicitly correlated local LCCSD-F12 method in which the basis set incompleteness error as well as the error caused by truncating the virtual orbital space to pair-specific local domains are strongly reduced.

J. Chem. Phys. **130**, 241101 (2009)

Production of O_2 Herzberg states in the deep UV photodissociation of ozone

R. Schinke, G. C. McBane, L. Shen, P. C. Singh, and **A. G. Suits**

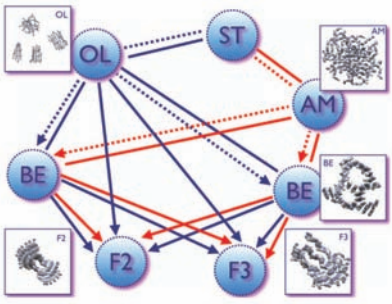


There are strong indications that the $O(^3P)+O_2$ products with very low kinetic energy release formed in the deep UV (226 nm) photodissociation of ozone reflect excitation of the Herzberg states of O_2—contradicting the earlier assignment to very high vibrational states.

J. Chem. Phys. **131**, 011101 (2009)

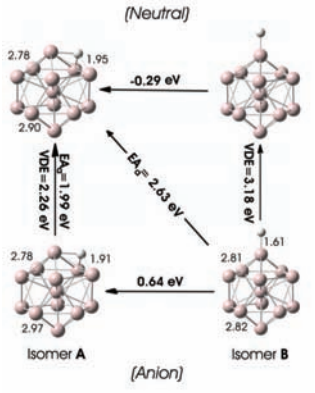
Diversity of kinetic pathways in amyloid fibril formation

Giovanni Bellesia and **Joan-Emma Shea**



The kinetics of peptide oligomerization was investigated using Langevin Dynamics simulations and a coarse-grained peptide model. The simulations show a rich diversity of aggregation pathways, modulated by the β–sheet propensity (flexibility) of the peptide.

J. Chem. Phys. **131**, 111102 (2009)



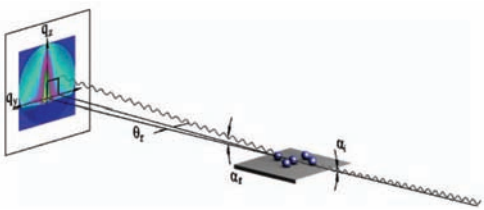
$Al_{13}H^-$: Hydrogen atom site selectivity and the shell model

A. Grubisic, X. Li, S. T. Stokes, K. Vetter, G. F. Ganteför, K. H. Bowen, P. Jena, B. Kiran, R. Burgert, and **H. Schnöckel**

A combination of anion photoelectron spectroscopy and density functional theory calculations are used to explore the influence of the shell model on H atom site selectivity in $Al_{13}H^-$.

J. Chem. Phys. **131**, 121103 (2009)

Combined temperature-programmed reaction and *in situ* x-ray scattering studies of size-selected silver clusters under realistic reaction conditions in the epoxidation of propene



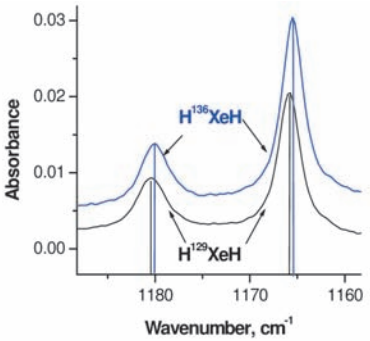
Stefan Vajda, Sungsik Lee, Kristian Sell, Ingo Barke, Armin Kleibert, Viola von Oeynhausen, Karl-Heinz Meiwes-Broer, Arantxa Fraile Rodríguez, Jeffrey W. Elam, Michael M. Pellin, Byeongdu Lee, Sönke Seifert, and **Randall E. Winans**

The catalytic activity and dynamical shape changes in size-selected nanoclusters are studied under realistic reaction conditions by using a combination of temperature-programmed reaction with *in situ* grazing-incidence small-angle x-ray scattering.

J. Chem. Phys. **131**, 121104 (2009)

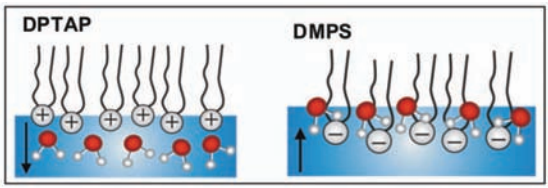
Direct visualization of the H–Xe bond in xenon hydrides: Xenon isotopic shift in the IR spectra

Vladimir I. Feldman, Alexey V. Kobzarenko, Irina A. Baranova, Alexander V. Danchenko, Fedor F. Sukhov, Ehud Tsivion, and **R. Benny Gerber**



Direct experimental evidence of isotopic shifts and complementary quantum calculations are presented for the H-Xe bond in HXeY type compounds.

J. Chem. Phys. **131**, 151101 (2009)



Observation of buried water molecules in phospholipid membranes by surface sum-frequency generation spectroscopy

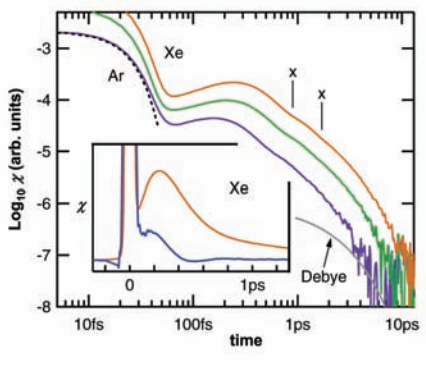
Maria Sovago, Erik Vartiainen, and **Mischa Bonn**

The structure and orientation of water molecules at the water-lipid interface is investigated using vibrational sum-frequency generation in conjunction with a maximum entropy phase retrieval method.

J. Chem. Phys. **131**, 161107 (2009)

Universal nonexponential relaxation: Complex dynamics in simple liquids

David A. Turton and **Klaas Wynne**



Using optical Kerr-effect spectroscopy, it is shown that for argon, krypton, and xenon, both the librational and diffusional contributions to the spectrum are surprisingly complex. The meaured behavior is shown to be similar to that observed for water, suggesting certain fundamental or universal properties in liquids.

J. Chem. Phys. **131**, 201101 (2009)

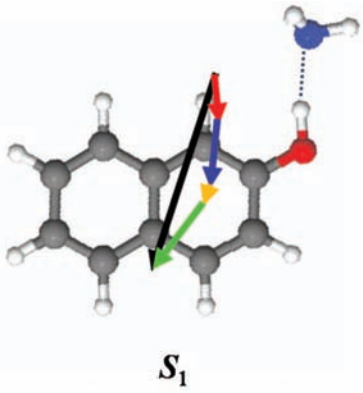
COMMUNICATIONS

Charge transfer by electronic excitation: Direct measurement by high resolution spectroscopy in the gas phase

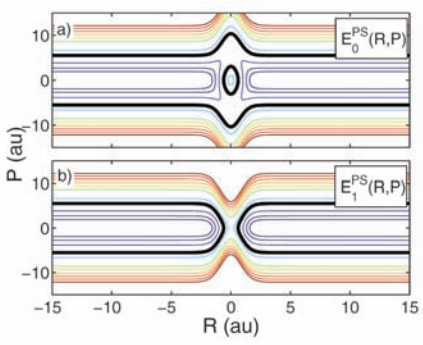
A. J. Fleisher, P. J. Morgan, and **D. W. Pratt**

The amount of charge transferred when a single ammonia complex of the photoacid β-naphthol (2HNA) is excited by light is reported. The measurement was made by comparing the permanent electric dipole moments of cis-2HNA in its ground (S_0) and excited (S_1) states, determined by Stark-effect studies of its fully resolved $S_1 \leftarrow S_0$ electronic spectrum.

J. Chem. Phys. **131**, 211101 (2009)



THEORETICAL METHODS AND ALGORITHMS



Phase-space surface hopping: Nonadiabatic dynamics in a superadiabatic basis

Neil Shenvi

The author constructs a phase-space surface hopping algorithm for use in systems that exhibit strong nonadiabatic coupling. For a simple model problem, phase-space surface hopping is shown to be more accurate than position-space surface hopping, especially when the nonadiabatic coupling is strong.

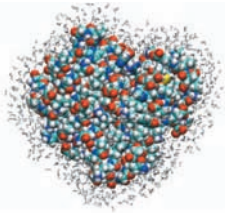
J. Chem. Phys. **130**, 124117 (2009)

Simulated x-ray scattering of protein solutions using explicit-solvent models

Sanghyun Park, Jaydeep P. Bardhan, Benoît Roux, and **Lee Makowski**

A novel formulation based on the atomistic description of water is presented in which scattering patterns are calculated from atomic coordinates of protein and water. Without any empirical adjustments, this method produces scattering patterns of unprecedented accuracy in the length scale between 5 and 100 Å.

J. Chem. Phys. **130**, 134114 (2009)



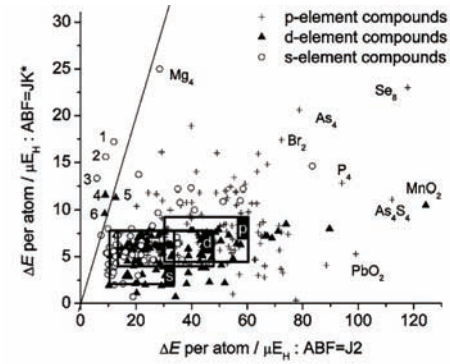
On the relation between time-dependent and variational density functional theory approaches for the determination of excitation energies and transition moments

Tom Ziegler, Michael Seth, Mykhaylo Krykunov, Jochen Autschbach, and **Fan Wang**

$$\begin{aligned}\rho'(1,1') &= \rho^{(0)}(1,1') + \Delta\rho'(1,1') \\ &= \rho^{(0)}(1,1') + \sum_{i}^{\text{occ}}\sum_{a}^{\text{vir}} U_{ai}\psi_i^*(1)\psi_a(1') \\ &+ \sum_{i}^{\text{occ}}\sum_{a}^{\text{vir}} U_{ai}^*\psi_a^*(1)\psi_i(1) \\ &+ \sum_{a}^{\text{vir}}\sum_{b}^{\text{vir}}\sum_{i}^{\text{occ}} U_{ai}^*U_{bi}\psi_a^*(1)\psi_b(1') \\ &- \sum_{i}^{\text{occ}}\sum_{k}^{\text{vir}}\sum_{a}^{\text{vir}} U_{ak}^*U_{ai}\psi_i^*(1)\psi_k(1') + O^{(3)}[U].\end{aligned}$$

The authors show it is possible to derive the basic eigenvalue equation of adiabatic time-dependent density functional theory within the Tamm–Dancoff approximation from a variational principle.

J. Chem. Phys. **130**, 154102 (2009)



Approximated electron repulsion integrals: Cholesky decomposition versus resolution of the identity methods

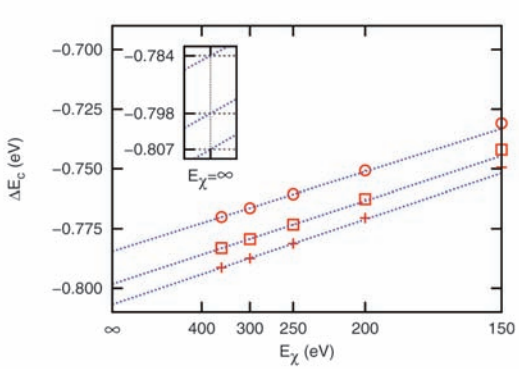
Florian Weigend, Marco Kattannek, and **Reinhart Ahlrichs**

The authors compare two procedures to gain efficiency by approximating two-electron integrals in molecular electronic structure calculations. "Resolution of the identity" methods are superior in speed, whereas Cholesky decomposition methods have certain advantages for extended basis sets.

J. Chem Phys. **130**, 164106 (2009)

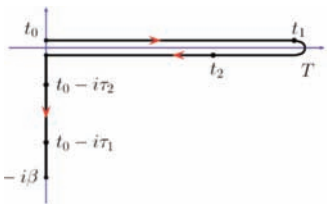
Second-order Møller–Plesset perturbation theory applied to extended systems. I. Within the projector-augmented-wave formalism using a plane wave basis set

M. Marsman, A. Grüneis , J. Paier, and **G. Kresse**



The authors present an implementation of the canonical formulation of second-order Møller–Plesset (MP2) perturbation theory within the projector-augmented-wave method under periodic boundary conditions using a plane wave basis set.

J. Chem. Phys. **130**, 184103 (2009)



Time propagation of the Kadanoff–Baym equations for inhomogeneous systems

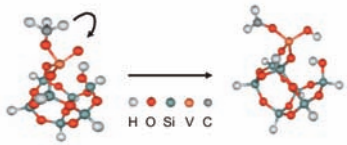
Adrian Stan, Nils Erik Dahlen, and **Robert van Leeuwen**

The authors present a time-propagation scheme for the Kadanoff–Baym equations for general inhomogeneous systems. These equations describe the time evolution of the nonequilibrium Green function for interacting many-body systems in the presence of time-dependent external fields.

J. Chem. Phys. **130**, 224101 (2009)

Transition state-finding strategies for use with the growing string method

Anthony Goodrow, Alexis T. Bell, and **Martin Head-Gordon**

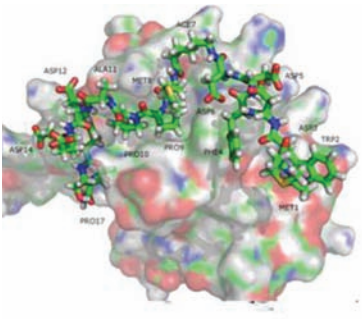


The authors develop three transition state-finding search algorithms to complement the speedup of the modified-growing string method: (1) a hybrid strategy, (2) an energy-weighted strategy, and (3) a substring strategy.

J. Chem. Phys. **130**, 224108 (2009)

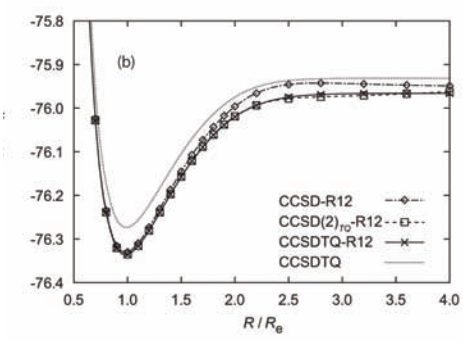
Probing hot spots on protein-protein interfaces with all-atom free-energy simulation

Irene Meliciani, Konstantin Klenin, Timo Strunk, Katja Schmitz, and **Wolfgang Wenzel**



Computational alanine screening has been developed for the prediction of hot spots based on existing structural information.

J. Chem. Phys. **131**, 034114 (2009)



Explicitly correlated combined coupled-cluster and perturbation methods

Toru Shiozaki, Edward F. Valeev, and **So Hirata**

Coupled-cluster methods have been extended to include the basis functions that explicitly depend on interelectronic distances in the wave function expansions with the aim of dramatically accelerating the basis-set convergence of correlation energies.

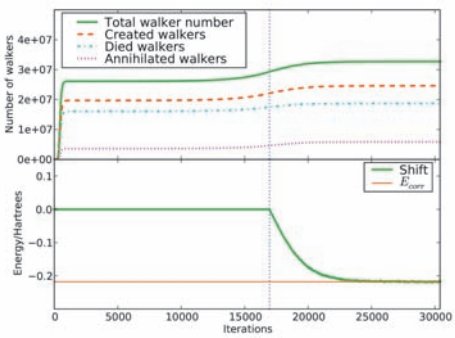
J. Chem. Phys. **131**, 044118 (2009)

Fermion Monte Carlo without fixed nodes: A game of life, death, and annihilation in Slater determinant space

George H. Booth, Alex J. W. Thom, and **Ali Alavi**

The authors have developed a new quantum Monte Carlo method for the simulation of correlated many-electron systems in full configuration-interaction spaces.

J. Chem. Phys. **131**, 054106 (2009)

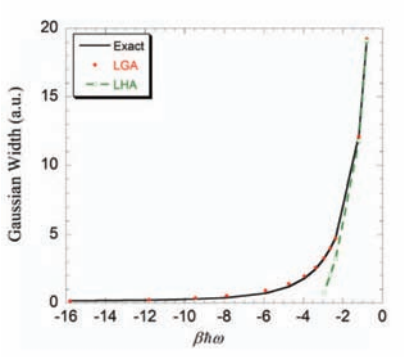


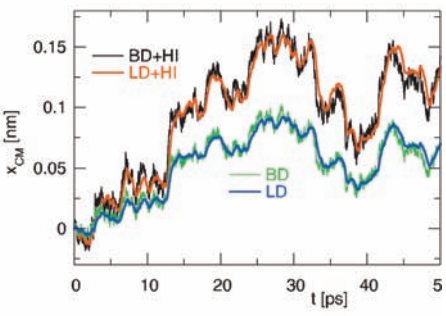
A simple model for the treatment of imaginary frequencies in chemical reaction rates and molecular liquids

Jian Liu and **Willian H. Miller**

A simple model for treating local imaginary frequencies that are important in the study of quantum effects in chemical reactions and various dynamical processes in molecular liquids is presented.

J. Chem. Phys. **131**, 074113 (2009)





Coarse grained simulations of a small peptide: Effects of finite damping and hydrodynamic interactions

Uwe Winter and **Tihamér Geyer**

The authors show that an analytic integration of the equations of damped motion with hydrodynamic interactions between the particles leads to a fast multiparticle propagation scheme, which captures short-time and short-range solvent effects.

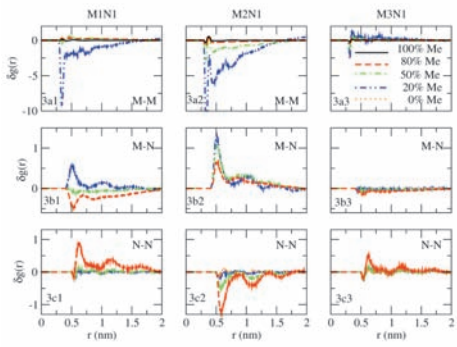
J. Chem. Phys. **131**, 104102 (2009)

Extended ensemble approach for deriving transferable coarse-grained potentials

J. W. Mullinax and **W. G. Noid**

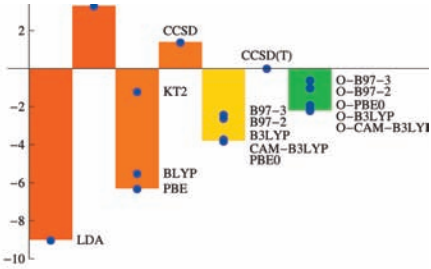
An extended ensemble framework for calculating transferable coarse-grained potentials that accurately reproduce the structure of atomistic models for multiple systems is presented.

J. Chem. Phys. **131**, 104110 (2009)



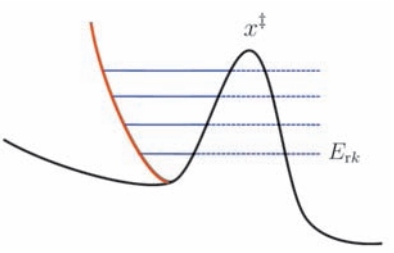
Benchmarking density-functional-theory calculations of rotational g tensors and magnetizabilities using accurate coupled-cluster calculations

Ola B. Lutnæs, Andrew M. Teale, Trygve Helgaker, David J. Tozer, Kenneth Ruud, and **Jürgen Gauss**



An accurate set of benchmark rotational g tensors and magnetizabilities are calculated using coupled-cluster singles-doubles theory and coupled-cluster single-doubles-perturbative-triples theory, in a variety of basis sets consisting of (rotational) London atomic orbitals.

J. Chem. Phys. **131**, 144104 (2009)



The ring-polymer molecular dynamics rate-theory in the deep-tunneling regime: Connection with semiclassical instanton theory

Jeremy O. Richardson and **Stuart C. Althorpe**

The ring-polymer molecular dymanics method is demonstrated to be equivalent to an automated and approximate implemenation of the "Im F" version of semiclassical instanton theory when used to calculate reaction rates in the deep-tunneling regime.

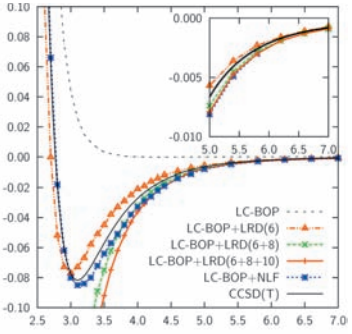
J. Chem. Phys. **131**, 214106 (2009)

Density functional method including weak interactions: Dispersion coefficients based on the local response approximation

Takeshi Sato and **Hiromi Nakai**

The authors propose a new method to calculate the atom-atom dispersion coefficients in a molecule for use in density functional theory with dispersion correction. This local response dispersion method is able to calculate the dispersion energy from the ground-state electron density.

J. Chem. Phys. **131**, 224104 (2009)



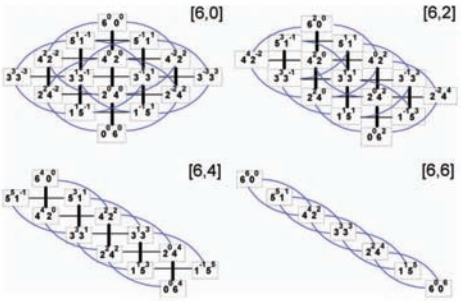
THEORETICAL METHODS AND ALGORITHMS

Critical points bifurcation analysis of high-ℓ bending dynamics in acetylene

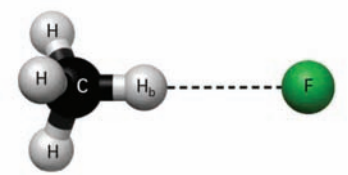
Vivian Tyng and **Michael E. Kellman**

The bending dynamics of acetylene with pure vibrational angular momentum excitation and nonzero quantum number ℓ are analyzed through the method of critical points analysis to find new anharmonic modes born in bifurcations of the low energy normal modes.

J. Chem. Phys. **131**, 244111 (2009)



GAS PHASE DYNAMICS



Accurate *ab initio* potential energy surface, dynamics, and thermochemistry of the $F+CH_4 \rightarrow HF+CH_3$ reaction

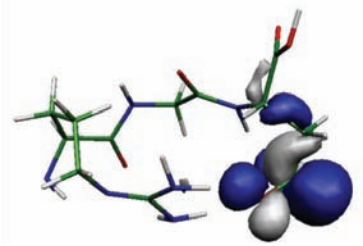
Gábor Czakó, Benjamin C. Shepler, Bastiaan J. Braams, and **Joel M. Bowman**

The reaction dynamics of the gas-phase reaction between a fluorine atom and a methane molecule are studied, and an accurate 12-dimensional potential energy surface (PES) is developed based on 19,384 *ab initio* energy points. Quasiclassical trajectory calculations of the reaction using the new PES are reported.

J. Chem. Phys. **130**, 084301 (2009)

The parent anion of the RGD tripeptide: Photoelectron spectroscopy and quantum chemistry calculations

Xiang Li, Haopeng Wang, Kit H. Bowen, G. Grégoire, F. Lecomte, Jean-Pierre Schermann, and **Charles Desfrançois**

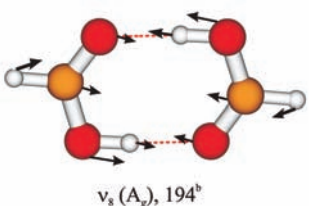


The gas-phase conformation of the intact parent unprotected RGD–peptide anion is investigated using a combination of anion photoelectron spectroscopy and quantum chemistry calculations of its low-energy stable structures.

J. Chem. Phys. **130**, 214301 (2009)

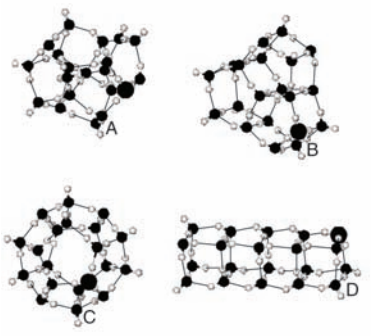
Probing the stiffness of the simplest double hydrogen bond: The symmetric hydrogen bond modes of jet-cooled formic acid dimer

Z. Xue and **M. A. Suhm**



Raman active fundamentals, overtones, and combination bands involving out-of-plane bending and stretching vibrations of the hydrogen bonds in jet-cooled formic acid dimer are reported. Preliminary experimental evidence for the most elusive fundamental vibration, symmetric OH torsion, is presented.

J. Chem. Phys. **131** 054301 (2009)



An *ab initio* study of the $(H_2O)_{20}H^+$ and $(H_2O)_{21}H^+$ water clusters

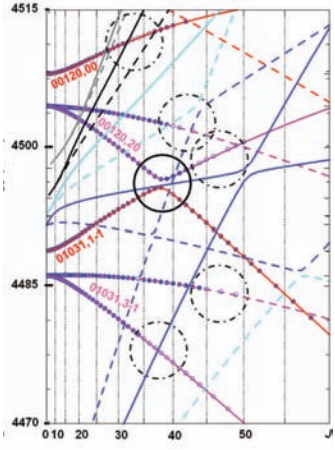
Tomasz Kuś, Victor F. Lotrich, Ajith Perera, and **Rodney J. Bartlett**

A study of the minimum Born–Oppenheimer structures of the protonated water clusters, $(H_2O)_nH^+$ for n=20 and 21. The results confirm that the lowest energy structure of the magic number n=21 clusters corresponds to a more stable form than that of the 20-mer clusters.

J. Chem. Phys. **131**, 104313 (2009)

Vibration-rotation pattern in acetylene. II. Introduction of Coriolis coupling in the global model and analysis of emission spectra of hot acetylene around 3 μm

Badr Amyay, Séverine Robert, Michel Herman, André Fayt, Balakrishna Raghavendra, Audrey Moudens, Jonathan Thiévin, Bertrand Rowe, and **Robert Georges**



A global model, updated as compared to previous work, allows all lines in the database to be simultaneously fitted, successfully. The updates are discussed taking into account, in particular, the systematic inclusion of Coriolis interaction.

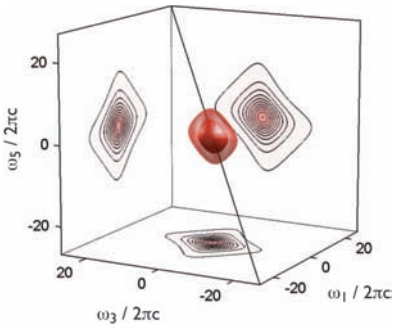
J. Chem. Phys. **131**, 114301 (2009)

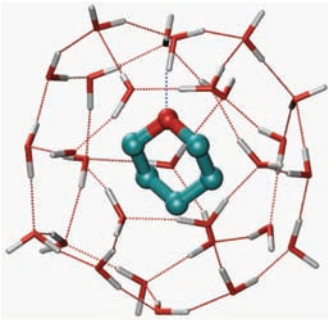
Purely absorptive three-dimensional infrared spectroscopy

Sean Garrett-Roe and **Peter Hamm**

Three-dimensional fifth-order vibrational infared spectroscopy is described. The measured spectra agree very well with simulations of the data based on the cumulant expansion.

J. Chem. Phys. **130**, 164510 (2009)





Linking microscopic guest properties to macroscopic observables in clathrate hydrates: Guest-host hydrogen bonding

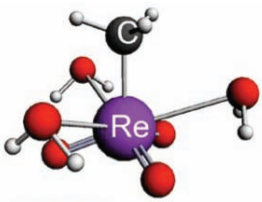
Saman Alavi, Robin Susilo, and **John A. Ripmeester**

The authors use molecular dynamics simulations to compare the properties of clathrate hydrates with cyclopentane, tetrahydrofuran (THF), 1,3-dioxolane, tetrahydropyran (THP), and p-dioxane as guests. Significant differences are observed between structural parameters and rotational dynamics for the different guests and related to the formation of guest-host hydrogen bonds in some (THF and THP) and the absence of similar hydrogen bonds in the clathrate hydrates of the other guests.

J. Chem. Phys. **130**, 174501 (2009)

Local structure of reaction intermediates probed by time-resolved x-ray absorption near edge structure spectroscopy

G. Smolentsev, G. Guilera, M. Tromp, S. Pascarelli, and **A. V. Soldatov**

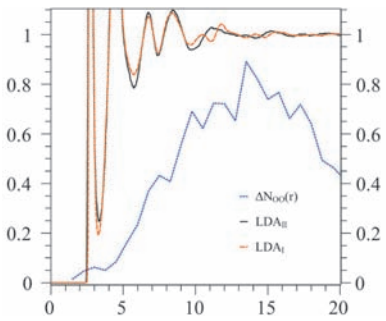


The proposed method combines principal component analysis of the series of experimental spectra, multidimensional interpolation of theoretical XANES as a function of structural parameters, and *ab initio* XANES calculations.

J. Chem. Phys. **130**, 174508 (2009)

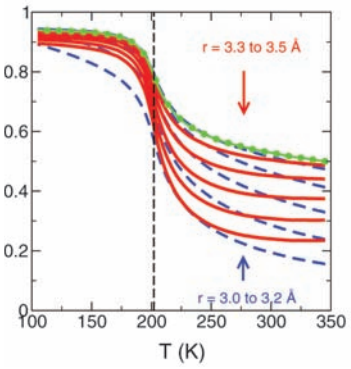
Relaxation effects in low density amorphous ice: Two distinct structural states observed by neutron diffraction

K. Winkel, D. T. Bowron, T. Loerting, E. Mayer, and **J. L. Finney**



The structure of low density amorphous ice, produced from high density amorphous ice by isobaric warming and very high density amporphous ice by isothermal decompression, are investigated via neutron diffraction with H/D isotopic substitution.

J. Chem. Phys. **130**, 204502 (2009)



Growing correlation length in supercooled water

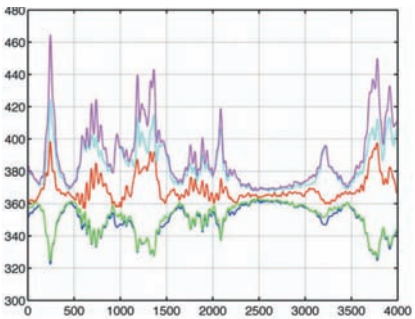
Emily B. Moore and **Valeria Molinero**

The evolution of the structure of water from the stable liquid to its glass, the low–density amorphous ice, at the critical cooling rate for vitrification is studied by molecular dynamics. A continuous transition to a tetrahedrally ordered low-density liquid is observed at 50 K below the temperature of maximum density and 25 K above a temperature of minimum density. The liquid-liquid transition temperature coincides with the maximum rate of change in the local structure.

J. Chem. Phys. **130**, 244505 (2009)

Ultrafast H_2 and D_2 rotational Raman responses in near critical CO_2: An experimental and theoretical study of anisotropic solvation dynamics

J. Peng, T. C. Castonguay, D. F. Coker, and **L. D. Ziegler**

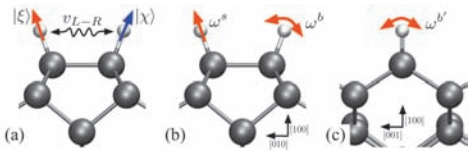


The optical heterodyne detected anisotropic rotational Raman responses of H_2 and D_2 in a near critical CO_2 solution are reported.

J. Chem. Phys. **131**, 054501 (2009)

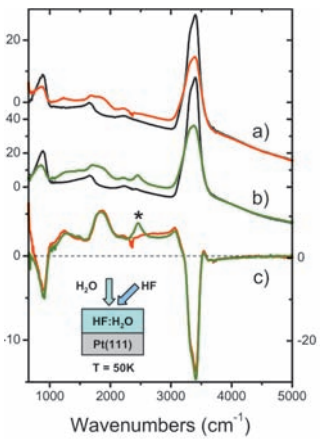
Isotope effects in the vibrational lifetime of hydrogen on germanium(100): Theory and experiment

Sung Sakong, Peter Kratzer, Xu Han, Thorsten Balgar, and **Eckart Hasselbrink**



Combining first-principles calculations and sum-frequency generation spectroscopy, the authors elucidate the microscopic details in the relaxation of the stretching vibration of hydrogen adsorbed on Ge(100).

J. Chem. Phys. **131**, 124502 (2009)



Dissociative adsorption of hydrogen fluoride onto amorphous solid water

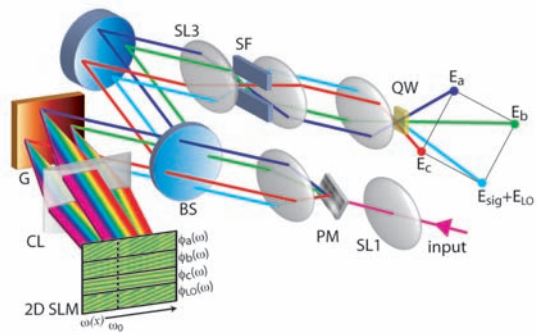
Patrick Ayotte, Zohreh Rafiei, François Porzio, and **Patrick Marchand**

Hydrogen fluoride is shown to be extensively ionically dissociated upon its adsorption onto and its dissolution within amorphous solid water films at 50 K. The results suggest a re-examination of dielectric and transport properties of HF-doped ice–including atmospheric processes involving this important halogen reservoir species.

J. Chem. Phys. **131**, 124517 (2009)

Three-dimensional electronic spectroscopy of excitons in GaAs quantum wells

Daniel B. Turner, Katherine W. Stone, Kenan Gundogdu, and **Keith A. Nelson**



The phase stability of four fully phase-coherent fields that are controlled using a spatiotemporal femtosecond pulse shaper is exploited to create 3D Fourier transform electronic spectral solids through a four-wave-mixing process in GaAs quantum wells.

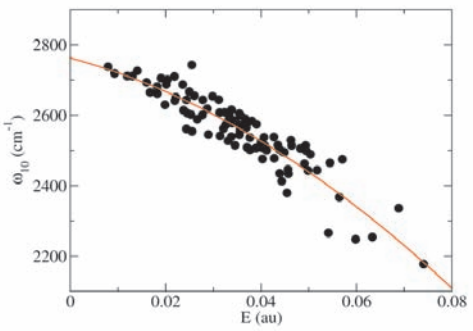
J. Chem. Phys. **131**, 144510 (2009)

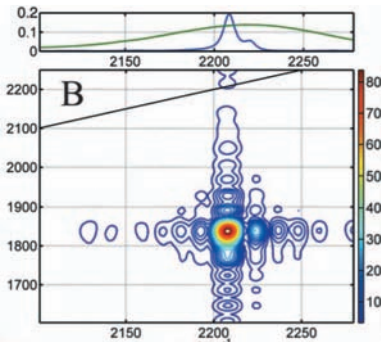
Water structure, dynamics, and vibrational spectroscopy in sodium bromide solutions

Y.-S. Lin, B. M. Auer, and **J. L. Skinner**

A theoretical study of steady-state and ultrafast vibrational spectroscopy, in the OD-stretch region, of dilute HOD in aqueous solutions of sodium bromide is presented where new spectroscopic maps are developed to undertake the study.

J. Chem. Phys. **131**, 144511 (2009)





Energy transport via coordination bonds

Valeriy M. Kasyanenko, Zhiwei Lin, Grigory I. Rubtsov, James P. Donahue, and **Igor V. Rubtsov**

The energy transport across coordination bonds in tetraethylammonium bis(maleonitriledithiolate) iron(III)nitrosyl complex, is investigated using dual-frequency RA 2DIR spectroscopy. A simple modeling of the energy transport is presented.

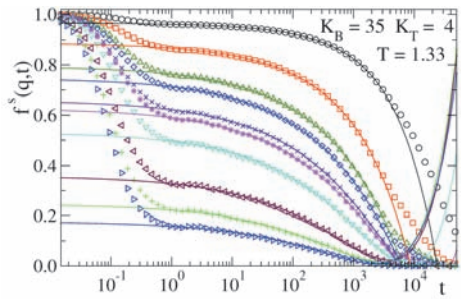
J. Chem. Phys. **131**, 154508

The role of intramolecular barriers on the glass transition of polymers: Computer simulations versus mode coupling theory

Marco Bernabei, Angel J. Moreno, and **Juan Colmenero**

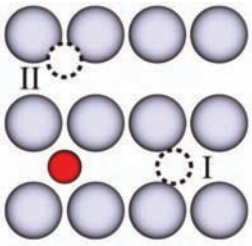
By systematically tuning the strength of the barriers, the authors investigate their role on the glass transition. Dynamic observables are analyzed within the framework of the mode coupling theory.

J. Chem. Phys. **131**, 204502 (2009)



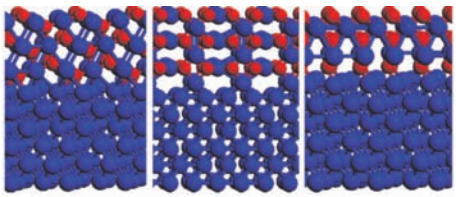
Vibrational mode-specific bond dissociation in a single molecule

J. R. Hahn and **W. Ho**



Tunneling electrons from a scanning tunneling microscope were used to image and dissociate single O_2-water-O complexes adsorbed on a Ag(110) surface at 13 K. The dissociation rate increases by ~100 times when the electron energy is equivalent to that of an O–H stretch.

J. Chem. Phys. **131**, 044706 (2009)



A first-principles study of bulk oxide formation on Pd(100)

Nicola Seriani, Judith Harl, Florian Mittendorfer, and **Georg Kresse**

The results give a framework for the interpretation of experiments of Pd oxide growth, showing the most stable orientation of the oxide film. A simple model employing density-functional theory energies predicts a Stranski–Krastanov growth mode for the oxide film.

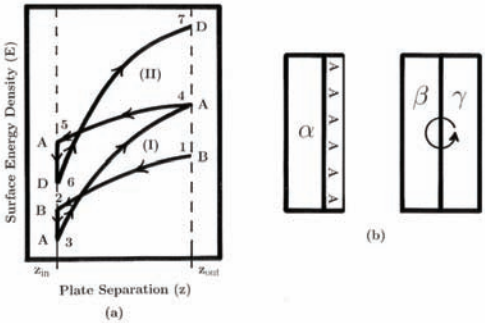
J. Chem. Phys. **131**, 054701 (2009)

Casimir chemistry

D. P. Sheehan

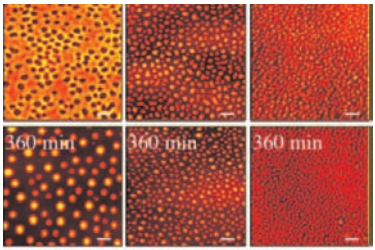
At the nanoscale, the Casimir effect can be used to mechanically tune critical aspects of chemical reactions by varying the spacing and composition of reaction vessel boundaries.

J. Chem. Phys. **131**, 104706 (2009)



Time-resolved specular and off-specular neutron reflectivity measurements on deuterated polystyrene and poly(vinyl methyl ether) blend thin films during dewetting process

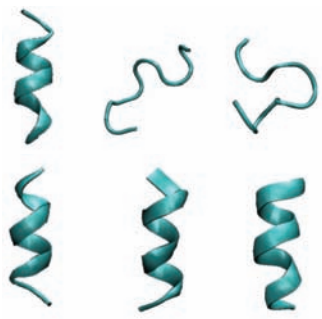
Hiroki Ogawa, Toshiji Kanaya, Koji Nishida, Go Matsuba, Jaroslaw P. Majewski, and **Erik Watkins**



Off-specular reflectivity was analyzed, for the first time, to evaluate kinetics of structure formation in the film plane during the dewetting process, showing that the droplets formation in micrometer scale occurred in the late stage of dewetting.

J. Chem. Phys. **131**, 104907 (2009)

BIOLOGICAL MOLECULES, BIOPOLYMERS & BIOLOGICAL SYSTEMS



Effect of trehalose on amyloid β (29–40)-membrane interaction

Allam S. Reddy, Aslin Izmitli, and **J. J. de Pablo**

The authors show that the insertion of amyloid β peptide into a membrane is more favorable when the peptide is folded into an α–helix than in a random coil conformation, suggesting that trehalose promotes the insertion of α–helical amyloid β into biological membranes.

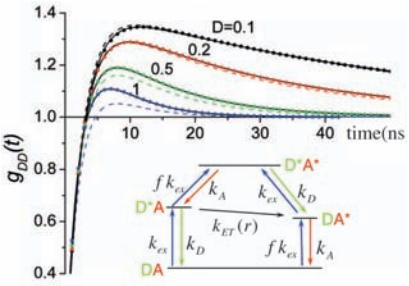
J. Chem. Phys. **131**, 085101 (2009)

Protein dynamics from single-molecule fluorescence intensity correlation functions

Irina V. Gopich, Daniel Nettels, Benjamin Schuler, and **Attila Szabo**

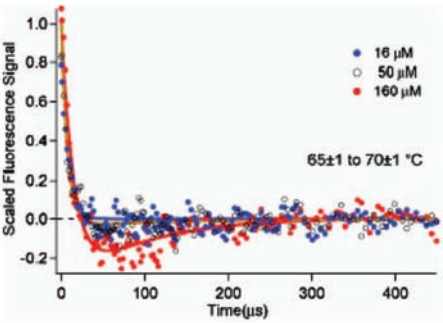
The authors propose and implement a simple procedure to analyze fluorescence intensity correlation functions measured in the presence of resonance energy transfer.

J. Chem. Phys. **131**, 095102 (2009)



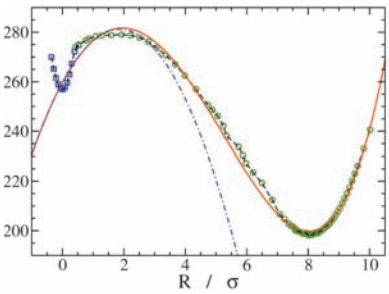
The transition state transit time of WW domain folding is controlled by energy landscape roughness

Feng Liu, Marcelo Nakaema, and **Martin Gruebele**



The duration τ_m of the molecular phase measured provides the best current estimate for the transit time from folded to unfolded state of a single protein molecule. The authors confirm this by directly comparing relaxation and single molecule signals computed by using Langevin trajectory models.

J. Chem. Phys. **131**, 195101 (2009)



Free energies of stable and metastable pores in lipid membranes under tension

Wouter K. den Otter

The free energy profile of pore formation in a lipid membrane has been calculated by molecular dynamics simulations with a coarse-grained lipid model. Details are provided of the simulation approach, which combines the potential of mean constraint force method with a reaction coordinate based on the local lipid density.

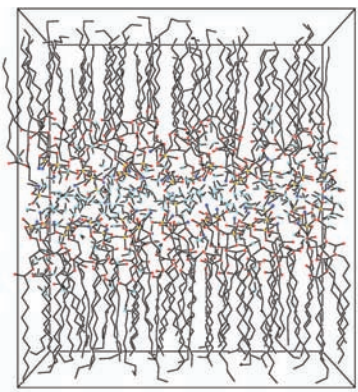
J. Chem. Phys. **131**, 205101 (2009)

Computer simulation of water-mediated forces between gel-phase phospholipid bilayers

Alexander Pertsin, Ivan Fedyanin, and **Michael Grunze**

Water-mediated forces between gel-phase phospholipid bilayers were calculated as a function of interbilayer separation using the grand canonical Monte Carlo technique and all-atom CHARMM force field.

J. Chem. Phys. **131**, 215102 (2009)



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