The Journal of Chemical Physics

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The Journal of Chemical Physics

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The Journal of Chemical Physics

2010 Editors' Choice

he 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 2010 that present groundbreaking research. This collection represents only a small fraction of the critical research published in JCP in 2010 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 2011.

COMMUNICATIONS

Ab initio dynamics of rare thermally activated reactions

S. a Beccara, G. Garberoglio, P. Faccioli, and F. Pederiva

This method is based on the path integral representation for the stochastic dynamics and yields the time evolution of both nuclear and electronic degrees of freedom, along the most probable reaction pathways, without spending computational time to explore metastable states. As a first illustrative



application, the authors characterize the dominant pathway in the cyclobutene \rightarrow butadiene reaction, using the semiempirical Parametrized Model 3 (PM3) approach.

J. Chem. Phys. 132, 111102 (2010)



The electronic spectrum of Li(NH₃)₄ L. Varriale, N. M. Tonge, N. Bhalla, and A. M. Ellis

This paper reports on the first electronic spectrum of $Li(NH_3)_4$ in the gas phase, which

was recorded using mass-selective depletion spectroscopy. The broad and structured spectrum confirms a recent theoretical prediction that the electronic spectrum of $\text{Li}(\text{NH}_3)_4$ will strongly overlap with the spectrum of the solvated electron in lithium-ammonia solutions.

J. Chem. Phys. 132, 161101 (2010)

COMMUNICATIONS

Exceptions to the *d*-band model of chemisorption on metal surfaces: The dominant role of repulsion between adsorbate states and metal *d*-states H. Xin and S. Linic

Shown here is a family of adsorbate-substrate systems that do not follow the trends in adsorption energies predicted by the *d*-band model. A physically transparent model is used to analyze this phenomenon. It was found that these adsorbate-substrate pairs are characterized by the repulsive interaction of the substrate *d*-band with the renormalized adsorbate states.



J. Chem. Phys. 132, 221101 (2010)

Accurate and efficient approximations to explicitly correlated coupledcluster singles and doubles, CCSD-F12 C. Hättig, D. P. Tew, and A. Köhn

Method	Noniterative	Iterative
CCSD	∞nN^4	$\infty n^2 N^4$
CCSD-F12a	$\infty n(N+X)^2 N^2$	$\infty n^2 N^4$
CCSD-F12b	$\infty n^2 N^4$	$\infty n^2 N^4$
CCSD(2) _{F12}	$\infty n^2 N^3 (N+X)$	$\infty n^2 N^4$
CCSD[F12]	$\infty n^2 N^3 (N+X)$	$\infty n^2 N^4$
CCSD(F12*)	$\infty n^2 N^3 (N+X)$	$\infty n^2 N^4$
CCSD(F12)	$\infty n^2 N^3 (N+X)$	$\infty n^2 N^3 (N+X)$

The explicitly correlated coupled-cluster singles and doubles CCSD-F12 method returns near basis set limit CCSD energies using only double- or triple- ζ orbital basis sets. However, the additional computational cost of the F12 contributions to the amplitude equations is considerable, which renders this method impractical for general applications. In this article, a new model CCSD(F12) is communicated, which has a computational cost close to that of conventional CCSD, while retaining the accuracy of CCSD(F12).

J. Chem. Phys. 132, 231102 (2010)

51

COMMUNICATIONS

The ionization and dissociation energies of HD

D. Sprecher, J. Liu, C. Jungen, W. Ubachs, and F. Merkt

The adiabatic ionization energy and the dissociation energy of HD have been determined using a hybrid experimental-theoretical method. Combining measurements with highly accurate theoretical values of the ionization energies of the one-electron systems H, D, and HD⁺ further enabled a new determination of the dissociation energy of HD.

J. Chem. Phys. 133, 111102 (2010)



Heavy Rydberg states: The H⁺H⁻ system A. Kirrander

Heavy Rydberg states are analogs of electronic Rydberg states, but with the electron replaced by a much heavier ion. The authors calculate *ab initio* the extremely long-range vibrational H^+H^- heavy Rydberg states in H_2 , and compare these to recent experiments. The calculated resonance positions and widths agree well with

experiment, but authors predict additional sharp interloper resonances corresponding to vibrational states trapped inside the barrier on potential energy curve $7 \, {}^{1}\Sigma_{o}^{+}$.

J. Chem. Phys. 133, 121103 (2010)



Ring polymer molecular dynamics beyond the linear response regime: Excess electron injection and trapping in liquids A. R. Menzeleev and T. F. Miller

Ring polymer molecular dynamics is used to simulate the dynamics of excess electron injection into fluid helium and liquid water. A method for modulating the initial energy of the excess electron is presented, and used to study both low-energy (cold) and high-energy (hot) electron injections.

J. Chem. Phys. 132, 034106 (2010)





A consistent and accurate *ab initio* parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu

S. Grimme, J. Antony, S. Ehrlich, and H. Krieg

This work refines the method of dispersion correction as an add-on to standard Kohn–Sham density functional theory (DFI-D), regarding higher accuracy, broader range of applicability, and less empiricism. The main new ingredients are atom-pairwise specific dispersion

coefficients and cutoff radii that are both computed from first principles. System (geometry) dependent information is used for the first time in a DFT-D type approach by employing the new concept of fractional coordination numbers.

J. Chem. Phys. 132, 154104 (2010)

High-order expansion of $T_2 \times t_2$ Jahn–Teller potential-energy surfaces in tetrahedral molecules D. Opalka and W. Domcke

Methods from Jahn–Teller theory and invariant theory have been combined for the construction of analytic diabatic potential-energy surfaces of triply degenerate states in tetrahedral molecules. The potentials of a threefold degenerate electronic state of T_2 symmetry, subject to the $T_2 \times t_2$ or $T_2 \times (t_2+t_2)$ Jahn–Teller effect in a threedimensional or six-dimensional space of nuclear coordinates, respectively, are considered.

J. Chem. Phys. 132, 154108 (2010)



Effects of patch size and number within a simple model of patchy colloids

A. Giacometti, F. Lado, J. Largo, G. Pastore, and F. Sciortino

Computer simulation and integral equation methods are applied to patchy colloids, modeled as spheres whose surfaces are decorated with two opposite attractive caps. It is found that the gas-liquid critical point moves to lower densities and temperatures with decreasing coverage. A rich variety of structures in crystal and fluid phases are found as the patch size is varied.

J. Chem. Phys. 132, 174110 (2010)





A homogeneous nonequilibrium molecular dynamics method for calculating the heat transport coefficient of mixtures and alloys K. K. Mandadapu, R. E. Jones, and P. Papadopoulos

This work generalizes Evans' homogeneous nonequilibrium method for estimating heat transport coefficient to multispecies molecular

systems described by general multibody potentials. The proposed method, in addition to being compatible with periodic boundary conditions, is shown to satisfy all the requirements of Evans' original method, namely, adiabatic incompressibility of phase space, equivalence of the dissipative and heat fluxes, and momentum preservation.

J. Chem. Phys. 133, 034122 (2010)

Rung 3.5 density functionals B. G. Janesko





Kohn–Sham density functional theory. In these Rung 3.5 functionals, intermediate in complexity between the semilocal approximations of Rungs 1–3 and fully nonlocal Rung 4 approximations, the exchange-correlation energy density at a point depends linearly (rather than quadratically) on the nonlocal Kohn–Sham one-particle density matrix in a finite neighborhood around the point.

J. Chem. Phys. 133, 104103 (2010)



Imaging mesoscopic nuclear spin noise with a diamond magnetometer

C. A. Meriles, L. Jiang, G. Goldstein, J. S. Hodges, J. Maze, M. D. Lukin, and P. Cappellaro

A novel NMR probe is described using a

nitrogen-vacancy center in diamond as a magnetic sensor for nanoscale nuclear spin imaging and spectroscopy. Such a sensor is able to probe the fluctuations of the "classical" dipolar field due to a large number of neighboring nuclear spins in a densely protonated sample.

J. Chem. Phys. 133, 124105 (2010)

Density cumulant functional theory: First implementation and benchmark results for the DCFT-06 model

A. C. Simmonett, J. J. Wilke, H. F. Schaefer, III, and W. Kutzelnigg

This work implements density cumulant functional theory for the first time. Benchmark results are provided for atoms and diatomic molecules, demonstrating the performance of DCFT-06 for both nonbonded and bonded interactions.

J. Chem. Phys. 133, 174122 (2010)



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2 • 0 • 1 • 0 EDITORS' CHOICE

Application of second-order Møller–Plesset perturbation theory with resolution-ofidentity approximation to periodic systems M. Katouda and S. Nagase

Electron correlation plays an important role in the accurate description of the conductive, optical, and magnetic properties of periodic systems. An efficient periodic boundary condition resolution-of-identity-MP2 method is developed here, based on the crystal orbital formalism and applicable to the calculations of large periodic systems. In this method, the slow convergence problem of lattice sum of long-range atomic orbital electron repulsion intervals in Fourier transformations was avoided by the use of Poisson and Gaussian mixed auxiliary basis functions.

J. Chem. Phys. 133, 184103 (2010)

Two-center integral evaluation: $T_{_{Pl}}^{\Theta m}$, $S_{_{Pl}}^{\Theta m}$, and $V_{_{Pl}}^{\Theta m}$
Fourier transformation of two-center integrals
Inversion of two-center integral matrix
Storage of the inverse matrix
Three-center integral evaluation: $\Gamma^{0,pq}_{p,pr}$ and $J^{0,pq}_{g,pr}$
1/3 index transformation: $\Gamma_{\mu,\mu\nu}^{rl=0,k,q} = \sum_{\mu p} \Gamma_{\mu,\mu\nu}^{l=0,pq} \left(C_{\mu\nu}^{k_l} \right)^* \exp(-ik_l p)$
and $J_{g,h^{*}}^{sk,q} = \sum_{\beta \mathbf{p}} J_{g,h^{*}}^{l=0,pq} \left(C_{\mu i}^{k_{i}} \right)^{*} \exp(-i\mathbf{k}_{i}\mathbf{p})$
2/3 index transformation: $\Gamma_{\mu,iu}^{\nu\mathbf{k},\mathbf{k}_{\nu}} = \sum_{v\mathbf{q}} \Gamma_{\mu,iv}^{\nu\mathbf{k},\mathbf{q}} C_{vu}^{\mathbf{k},\mathbf{q}} \exp(i\mathbf{k}_{u}\mathbf{q})$
and $J_{g,u}^{\sigma\mathbf{k},\mathbf{k}_u} = \sum_{\mathbf{q}} J_{g,u}^{\sigma\mathbf{k},\mathbf{q}} C_{cg}^{\mathbf{k}_u} \exp(i\mathbf{k}_u \mathbf{q})$
Storage of three-center integrals Γ^{*} and J^{*}
Reading of inverse matrix and three-center integrals $\ \Gamma^* \ $ and $\ J^*$
3/3 index transformation: $\begin{pmatrix} \mathbf{C}^* \\ \mathbf{D}^* \end{pmatrix} = \begin{pmatrix} \mathbf{T} & \mathbf{S} \\ \mathbf{S}^* & \mathbf{V} \end{pmatrix}^{-1} \begin{pmatrix} \mathbf{\Gamma}^* \\ \mathbf{J}^* \end{pmatrix}$
Storage of three-center integrals C'' and D''
Reading of three-center integrals $\ensuremath{\Gamma}'', \ensuremath{J}'', \ensuremath{C}'', \ensuremath{a}''$ and \ensuremath{D}''
Four-center CO integral generation: $\mathbf{Q} = \begin{pmatrix} \mathbf{C}^{r^{\dagger}} & \mathbf{D}^{r^{\dagger}} \end{pmatrix} \begin{pmatrix} \mathbf{\Gamma}^{s} \\ \mathbf{J}^{r} \end{pmatrix}$
MP2 correlation energy accumulation by eq. (3)

/=0 /=1 /=2

Total J representation



Uncoupled representation

Quantum theory of molecular collisions in a magnetic field: Efficient calculations based on the total angular momentum representation T. V. Tscherbul and A. Dalgarno

An efficient method is presented for

rigorous quantum calculations of atom-molecule and molecule-molecule collisions in a magnetic field. The method is based on the expansion of the wave function of the collision complex in basis functions with well-defined total angular momentum in the body-fixed coordinate frame.

J. Chem. Phys. 133, 184104 (2010)

Nonlocal van der Waals density functional: The simpler the better **O. A. Vvdrov and T. Van Voorhis**

The authors here devise a nonlocal correlation energy functional that describes the entire range of dispersion interactions in a seamless fashion using only the electron density as input. The new functional is considerably simpler than its predecessors of a similar type. The functional has a tractable and robust analytic form that lends itself to efficient self-consistent implementation. The functional proposed in this work is a computationally inexpensive electronic structure tool of broad applicability.



2

PKE (eV)



GAS PHASE DYNAMICS

(a) Signal (arb. unit) Signal (arb. unit) 1 0 -100 100 200 300 400 0 Delay (fs) 2 (b) 0 unit) 0.8 PKE (eV) 0.0 0.0 Signal (arb. u 1 0 L. -100 0 100 200 Delay (fs) 300 400

Time-resolved photoelectron imaging of ultrafast $S_2 \rightarrow S_1$ internal conversion through conical intersection in pyrazine Y.-I. Suzuki, T. Fuji, T. Horio, and T. Suzuki

A nonadiabatic electronic transition through a conical intersection was studied by pumpprobe photoelectron imaging spectroscopy with a 22 fs time resolution in the benchmark polyatomic molecule of pyrazine and deuterated pyrazine.

9

J. Chem. Phys. 132, 174302 (2010)

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GAS PHASE DYNAMICS

Photofragment angular momentum distributions in the molecular frame. II. Single state dissociation, multiple state interference, and nonaxial recoil in photodissociation of polyatomic molecules T. P. Rakitzis and A. J. Alexander



In this paper is presented an $a_q^k(s)$ polarization-

parameter model to describe product angular momentum polarization from the one-photon photodissociation of polyatomic molecules in the molecular frame. This model is applied to the linearly polarized polyatomic molecules and to dissociation mechanisms with nonaxial recoil and multiple state interference, giving insight into geometrical properties.

J. Chem. Phys. 132, 224310 (2010)



Valence photoelectron spectroscopy of N₂ and CO: Recoil-induced rotational excitation, relative intensities, and atomic orbital composition of molecular orbitals T. D. Thomas, E. Kukk, T. Ouchi, A. Yamada, H. Fukuzawa, K. Ueda, R. Püttner, I. Higuchi, Y. Tamenori, T. Asahina, N. Kuze, H. Kato, M. Hoshino, H. Tanaka, A. Lindblad, and L. J. Sæthre

Recoil-induced rotational excitation accompanying photoionization has been measured for the X, A, and B

states of N_2^+ and CO⁺ over a range of photon energies from 60 to 900 eV. These measurements provide a tool for investigating the atomic orbital composition of the molecular orbitals.

J. Chem. Phys. 133, 174312 (2010)

Dipole moment surface of the van der Waals complex CH₄-N₂

N. Zvereva-Loëte, Y. N. Kalugina, V. Boudon, M. A. Buldakov, and V. N. Cherepanov



The interaction-induced dipole moment surface of the van

der Waals CH_4 – N_2 complex has been calculated for a broad range of intermolecular separations *R* and configurations in the approximation of the rigid interacting molecules at the MP2 and CCSD(T) levels of theory using the correlation-consistent aug-cc-pVTZ basis set with the basis set superposition error correction.

J. Chem. Phys. **133**, 184302 (2010)

GAS PHASE DYNAMICS

Water binding sites in 2-*para*- and 2-*ortho*-fluorophenylethanol: A high-resolution UV experiment and *ab initio* calculations

R. Karaminkov, S. Chervenkov, and H. J. Neusser

The singly hydrated complexes of the flexible prototype molecules 2*para-* and 2-*ortho*-fluorophenylethanol have been investigated by combination of high-resolution resonance-enhanced two-photon ionization spectroscopy in a cold supersonic beam and quantum chemistry *ab initio* calculations. Conformational structures of the above complexes are identified, which correspond to water binding to the most stable gauche monomer's conformers in both cases.



J. Chem. Phys. 133, 194301 (2010)



Rotational dependence of the proton-transfer reaction HBr⁺ + CO₂ \rightarrow HOCO⁺ + Br. II. Comparison of HBr⁺ (² $\Pi_{3/2}$) and HBr⁺ (² $\Pi^{1/2}$) L. Paetow, F. Unger, B. Beutel, and K.-M. Weitzel

The effects of reactant ion rotational excitation on the exothermic proton-transfer reactions of HBr⁺(${}^{2}\Pi^{1/2}$) and DBr⁺(${}^{2}\Pi_{1/2}$), respectively, with CO₂ were studied in a guided ion beam apparatus. The reaction cross section decreases with increasing rotational energy, however, the dependence changes with collision energy.

J. Chem. Phys. 133, 234301 (2010)

Recombination-pumped triatomic hydrogen infrared lasers

R. J. Saykally, E. A. Michael, J. Wang, and C. H. Greene



Mid-infrared laser lines observed in

hydrogen/rare gas discharges are assigned to three-body recombination processes involving an electron, a rare gas (He or Ne) atom, and the triatomic hydrogen ion (H_3^+) . Calculations of radiative transitions between neutral H_3 Rydberg states support this interpretation, and link it to recent results for hydrogenic/rare gas afterglow plasmas.

J. Chem. Phys. 133, 234302 (2010)

2 • 0 • 1 • 0 EDITORS' CHOICE

CONDENSED PHASE DYNAMICS, STRUCTURE, & THERMODYNAMICS

Proton disorder and the dielectric constant of type II clathrate hydrates S. W. Rick and D. L. Freeman

Computational studies are presented examining the degree of proton disorder, the dielectric properties, and the molar volumes of sII clathrate hydrates with argon and H_2 in aqueous cages. The extent of proton disorder is found to be insensitive to the guest identity. The dielectric constants of clathrates are found to be smaller than that of ice, mainly due to the lower densities of the clathrate systems.





oblique mirror

inverse mirror

J. Chem. Phys. 132, 054509 (2010)



Calculations of vibrationally resonant sumand difference-frequency-generation spectra of chiral molecules in solutions: Three-wavemixing vibrational optical activity J.-H. Choi, S. Cheon, and M. Cho

Quantum chemistry calculations were carried out to obtain nonlinear optical properties for a representative chiral molecule, (*S*)-methyl lactate, and numerically simulate the corresponding spectra. It is shown that the circular polarization three-wave-mixing signal intensities are quantitatively similar to those of the linear polarization threewave-mixing signals, respectively, and that they are sensitive to the absolute configuration of chiral molecule.

J. Chem. Phys. 132, 074506 (2010)

An exciton scattering model for carrier multiplication in semiconductor nanocrystals: Theory A. Pirvatinski and K. A. Velizhanin

The effect of carrier multiplication in semiconductor nanocrystals is systematically treated by employing an exciton scattering approach. Using projection operators, the Coulomb coupled multiexciton dynamics is reduced to scattering dynamics in the space spanning both single- and biexciton states.

J. Chem. Phys. 133, 084508 (2010)



CONDENSED PHASE DYNAMICS, STRUCTURE, & THERMODYNAMICS

Product gas evolution above planar microstructured model catalysts— A combined scanning mass spectrometry, Monte Carlo, and Computational Fluid Dynamics study

M. Roos, J. Bansmann, D. Zhang, O. Deutschmann, and R. J. Behm

The transport and distribution of reaction products above catalytically active Pt microstructures was studied by spatially resolved scanning mass spectrometry in combination with Monte Carlo simulation and fluid dynamics calculations, using the oxidation of CO as test



reaction. Measurement and reaction conditions are defined where effects induced by the capillary tip can be neglected ('minimal invasive measurements') and provide a basis for the evaluation of catalyst activities on microstructured model systems.

J. Chem. Phys. 133, 094504 (2010)



Preferential solvation dynamics in liquids: How geodesic pathways through the potential energy landscape reveal mechanistic details about solute relaxation in liquids C. N. Nguyen and R. M. Stratt

The dynamics of preferential solvation, is studied for the geodesic paths in a simple atomic liquid mixture. The mechanism for preferential solvation features a reasonably sharp onset for slow diffusion, and that this diffusion involves a sequential, rather than concerted, series of solvent exchanges.

J. Chem. Phys. 133, 124503 (2010)

2 • 0 • 1 • 0 EDITORS' CHOICE

CONDENSED PHASE DYNAMICS, STRUCTURE & THERMODYNAMICS

Watching solvent friction impede ultrafast barrier crossings: A direct test of Kramers theory J. M. Anna and K. J. Kubarych

Two-dimensional infrared chemical exchange spectroscopy is used to systematically investigate how solvent dynamics influence activated barrier crossings on an electronic ground state. Use of the electronic ground state facilitates a direct comparison with Kramers theory of condensed phase reaction kinetics and avoids the significant complication of electronic excitation. For the first time, an electronic ground state with a well-defined transition state is directly probed in the time domain.



J. Chem. Phys. 133, 174506 (2010)

STRUCTURES, INTERFACES, AND MATERIALS





Fokker–Planck analysis of separation dependent potentials and diffusion coefficients in simulated microscopy experiments

D. J. Beltran-Villegas, R. M. Sehgal, D. Maroudas, D. M. Ford, and M. A. Bevan

The authors developed a Fokker–Planck (FP) formalism to simultaneously extract both particle-surface interaction potentials and position-dependent diffusion coefficients. Their results demonstrate the ability to extract both static and dynamic information from microscopy measurements of

isolated particles near surfaces, which provides a foundation for further investigation of particle ensembles and nonequilibrium systems.

J. Chem. Phys. 132, 044707 (2010)

STRUCTURES, INTERFACES, AND MATERIALS

Structure and infrared absorption of the first layer C_2H_2 on the NaCl(100) single-crystal surface

A. G. Cabello-Cartagena, J. Vogt, and H. Weiss

The adsorbate structure of the first layer acetylene on the NaCl(100) single-crystal surface is investigated using polarization infrared spectroscopy in combination with low-energy electron diffraction (LEED) experiments, and



potential calculations on the basis of pair potentials. Total energy minimizations support a new structure model which contains five inequivalent molecules per unit cell in a herringbone arrangement. The application of a vibrational exciton approach demonstrates that this new structure model can reproduce the triplet spectrum observed in the infrared experiments.

J. Chem. Phys. 132, 074706 (2010)



Direct and indirect electron transfer at a semiconductor surface with an adsorbate: Theory and application to Ag₃Si(111):H A. S. Leathers, D. A. Micha, and D. S. Kilin

A theoretical and computational study of photoinduced electron transfer between a metal cluster and a semiconductor surface is presented. Results obtained using electronic parameters from *ab initio* density functional calculations for the Ag₃Si(111):H system

photoexcited by visible light show that indirect electron transfer is a lot more likely than direct transfer and to lead to longer lasting electronic charge separation.

J. Chem. Phys. 132, 114702 (2010)

Observation of low heat capacities for vapor-deposited glasses of indomethacin as determined by AC nanocalorimetry K. L. Kearns, K. R. Whitaker, M. D. Ediger, H. Huth, and C. Schick



Alternating current nanocalorimetry was used to evaluate the heat capacity and kinetic stability of highly stable glass films of indomethacin (IMC) prepared by physical vapor deposition as a function of thickness. Interpretation of results indicate that the transformation of stable glass into supercooled liquid can occur by either a surface-initiated or bulk mechanism. In these experiments, the structural relaxation time of the IMC supercooled liquid was observed to be nearly independent of sample thickness.

J. Chem. Phys. 133, 014702 (2010)

STRUCTURES, INTERFACES, AND MATERIALS

Electronic effects of single H atoms on Ge(001) revisited

G. A. Shah, M. W. Radny, P. V. Smith, S. R. Schofield, and N. J. Curson

The adsorption of isolated H atoms on the Ge(001) surface is studied using density functional theory (DFT) and scanning tunnelling microscopy (STM). Two stable adsorption positions that are found in DFT correspond to H atom attachment to an up- or down-buckled Ge dimer atom, respectively. Surprisingly, in the case where H bonds



to the down-buckled Ge atom, it was found that there is a redistribution of a unit of charge which leaves the net charge of the doubly occupied dangling bond of the unreacted Ge atom intact.

J. Chem. Phys. 133, 014703 (2010)



Helium atom diffraction measurements of the surface structure and vibrational dynamics of CH₃–Si(111) and CD₃–Si(111) surfaces

J. S. Becker, R. D. Brown, E. Johansson, N. S. Lewis, and S. J. Sibener

The surface structure and vibrational dynamics of CH_3 – Si(111) and CD_3 –Si(111) surfaces were measured using helium atom scattering. The excellent quality of the observed diffraction patterns, along with minimal diffuse background,

indicated a high degree of long-range ordering and a low defect density for this interface. Experiments presented yield detailed information on the dynamical properties of these robust and technologically interesting semiconductor interfaces.

J. Chem. Phys. 133, 104705 (2010)

DFT+*U* study of defects in bulk rutile TiO₂ C. Hättig, D. P. Tew, and A. Köhn

Rutile titanium dioxide (titania) is the most studied transition metal oxide within surface science. Electronic gap states in defected titania are studied using the Hubbard-U approximation in the grid-based projector-



augmented wave density functional theory code. The defects considered are titanium interstitials, oxygen vacancies, and hydrogen dopants in the rutile phase of bulk titanium dioxide.

J. Chem. Phys. 133, 144708 (2010)

POLYMERS AND COMPLEX SYSTEMS

A numerical study of mobility in thin films of fullerene derivatives R. C. I. MacKenzie, J. M. Frost. and J. Nelson

Electron mobility in films of fullerene derivatives is investigated numerically by attaching aliphatic chains to the C⁶⁰ cage. Molecular dynamics is used to generate film morphology, quantum chemical methods to calculate intermolecular charge transfer rates, and Monte Carlo methods to



simulate time-of-flight experiments. It is found that as the length of the aliphatic side chain increases, the configurational disorder increases and thus the mobility decreases.

J. Chem. Phys. 132, 064904 (2010)



General approach to polymer chains confined by interacting boundaries K. F. Freed, J. Dudowicz, E. B. Stukalin, and J. F. Douglas

This article takes a general approach to describing polymers under conditions of weak to moderate confinement and applies this semianalytic method specifically to determine the thermodynamics and static structure factor for a flexible polymer confined between impenetrable interacting parallel plate boundaries.

J. Chem. Phys. 133, 094901 (2010)

2•0•1•0 EDITORS' CHOICE

BIOLOGICAL MOLECULES, BIOPOLYMERS, & BIOLOGICAL SYSTEMS

Coupling of twist and writhe in short DNA loops

S. Medalion, S. M. Rappaport, and Y. Rabin

In order to study the coupling between the writhe and twist distributions for various DNA lengths, Monte Carlo simulations were performed for wormlike rods. For sufficiently short DNA, the writhe distribution differs from that of a model with bending energy only. The simulation results are compared with a factorization approximation and experimental tests are proposed.

J. Chem. Phys. 132, 045101 (2010)



Nucleation theory with delayed interactions: An application to the early stages of the receptor-mediated adhesion/fusion kinetics of lipid vesicles

A. Raudino and M. Pannuzzo

This research reports on the development of semiquantitative theory aimed at describing the adhesion kinetics between soft objects, such as living cells or vesicles. In addition, the investigators look at the effect of the ligand-receptor pairing kinetics at the adhesion site in the time course of the patch expansion.

J. Chem. Phys. 132, 045103 (2010)

Effects of side-chain packing on the formation of secondary structures in protein folding

S. Yasuda, T. Yoshidome, H. Oshima, R. Kodama, Y. Harano, and M. Kinoshita





(d)

The entropy of water plays an important role in protein folding. This paper investigates the specific role that side-chain packing plays in increasing water entropy for α -helix and β -sheet secondary structures.

J. Chem. Phys. 132, 065105 (2010)







BIOLOGICAL MOLECULES, BIOPOLYMERS, & BIOLOGICAL SYSTEMS

Probing single nanometer-scale pores with polymeric molecular rulers S. E. Henrickson, E. A. DiMarzio, Q. Wang, V. M. Stanford, and J. J. Kasianowicz

This paper shows that polynucleotides can be used to probe structural features of the α -hemolysin channel. Specifically, both the pore length and channel aperture profile can be estimated. The results are consistent with the channel crystal structure and suggest that polymer-based "molecular rulers" may prove useful in deducing the structures of nanometer-scale pores in general.



J. Chem. Phys. 132, 135101 (2010)



DNA-protein binding rates: Bending fluctuation and hydrodynamic coupling effects

Y. von Hansen, R. R. Netz, and M. Hinczewski

Diffusion-limited reactions between a diffusing particle and a target site on a semiflexible polymer, a key factor determining the kinetics of DNA-protein binding and polymerization of cytoskeletal filaments,

are investigated. The theory presented focuses on two competing effects: polymer shape fluctuations, which speed up association, and the hydrodynamic coupling between the diffusing particle and the chain, which slows down association.

J. Chem. Phys. 132, 135103 (2010)

The electrostatics of solvent and membrane interfaces and the role of electronic polarizability

I. Vorobyov and T. W. Allen

The electrostatics of solvent and lipid bilayer interfaces are investigated with the aim of understanding the interaction of ions and charged peptides with biological membranes.

J. Chem. Phys. 132, 185101 (2010)



2 • 0 • 1 • 0 EDITORS' CHOICE

BIOLOGICAL MOLECULES, BIOPOLYMERS, & BIOLOGICAL SYSTEMS

Slow molecular dynamics close to crystal surfaces during crystallization of a protein lysozyme studied by fluorescence correlation spectroscopy S. Tanaka

Fluorescence correlation spectroscopy was applied to the crystallization processes of egg-white lysozyme to investigate the molecular dynamics less than one micron from crystal surfaces of both tetragonal single crystals and needlelike spherulites. The observations are explained as arising from aggregates of needlelike crystals that mature to form single crystals.



J. Chem. Phys. 133, 095103 (2010)





Atomistic theory of amyloid fibril nucleation R. Cabriolu, D. Kashchiev, and S. Auer

This work considers the nucleation of amyloid fibrils at the molecular level when the process takes place by a direct polymerization of peptides or protein segments into β -sheets. The analysis illustrates a unique feature of atomistic nucleation theory that the size of the fibril nucleus is a constant integer in a given supersaturation range. The results obtained are applicable to homogeneous nucleation, which occurs when the protein solution is sufficiently pure and/or strongly supersaturated.

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