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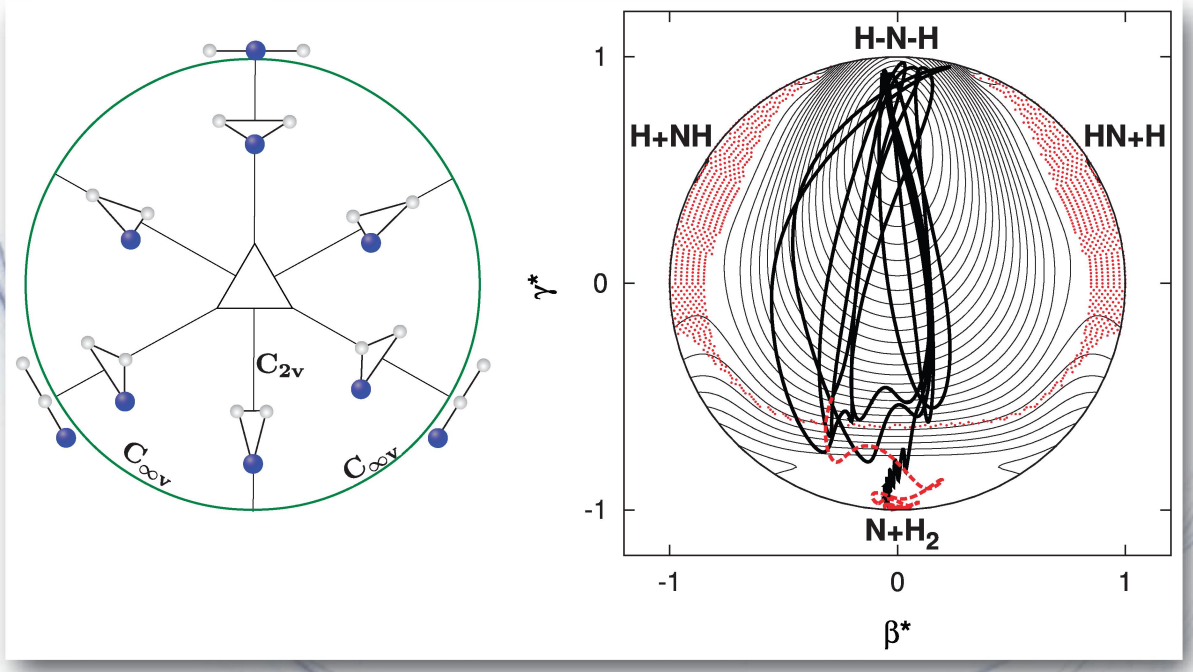

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COMMUNICATIONS

Communication: Water on hexagonal boron nitride from diffusion Monte Carlo
Yasmine S. Al-Hamdani, Ming Ma, Dario Alfè, O. Anatole von Lilienfeld and Angelos Michaelides
J. Chem. Phys. **142**, 181101 (2015); http://dx.doi.org/10.1063/1.4921106

ARTICLES

Theoretical Methods and Algorithms

On a theory of stability for nonlinear stochastic chemical reaction networks
Patrick Smadbeck and Yiannis N. Kaznessis
J. Chem. Phys. **142**, 184101 (2015); http://dx.doi.org/10.1063/1.4919834

Dynamically consistent method for mixed quantum-classical simulations: A semiclassical approach
Sergey V. Antipov, Ziyu Ye and Nandini Ananth
J. Chem. Phys. **142**, 184102 (2015); http://dx.doi.org/10.1063/1.4919667

Stochastic lumping analysis for linear kinetics and its application to the fluctuation relations between hierarchical kinetic networks
De-Ming Deng and Cheng-Hung Chang
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Ensemble density functional theory method correctly describes bond dissociation, excited state electron transfer, and double excitations
Michael Filatov, Miquel Huix-Rotllant and Irene Burghardt
J. Chem. Phys. **142**, 184104 (2015); http://dx.doi.org/10.1063/1.4919773

A very general rate expression for charge hopping in semiconducting polymers
Rocco P. Fornari, Juan Aragó and Alessandro Troisi
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Density-functional errors in ionization potential with increasing system size
Sarah R. Whittleton, Xochitl A. Sosa Vazquez, Christine M. Isborn and Erin R. Johnson
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Semi-stochastic full configuration interaction quantum Monte Carlo: Developments and application
N. S. Blunt, Simon D. Smart, J. A. F. Kersten, J. S. Spencer, George H. Booth and Ali Alavi
J. Chem. Phys. **142**, 184107 (2015); http://dx.doi.org/10.1063/1.4920975

Advanced Experimental Techniques

A unified heteronuclear decoupling strategy for magic-angle-spinning solid-state NMR spectroscopy
Asif Equbal, Morten Bjerring, P. K. Madhu and Niels Chr. Nielsen
J. Chem. Phys. **142**, 184201 (2015); http://dx.doi.org/10.1063/1.4919634

Atoms, Molecules, and Clusters

Structure and spectroscopic properties of neutral and cationic tetratomic [C,H,N,Zn] isomers: A theoretical study
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J. Chem. Phys. **142**, 184301 (2015); http://dx.doi.org/10.1063/1.4919879

The effect of intersystem crossings in $N(^2D) + H_2$ collisions

B. R. L. Galvão and L. A. Poveda
J. Chem. Phys. **142**, 184302 (2015); http://dx.doi.org/10.1063/1.4919743

Electronic spectra and excited state dynamics of pentafluorophenol: Effects of low-lying πσ* states
Shreetama Karmakar, Deb Pratim Mukhopadhyay and Tapas Chakraborty
J. Chem. Phys. **142**, 184303 (2015); http://dx.doi.org/10.1063/1.4919950

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J. Chem. Phys. **142**, 184304 (2015); http://dx.doi.org/10.1063/1.4919692

Jet cooled cavity ringdown spectroscopy of the A˜2E″←X˜2A′2 transition of the NO_3 radical
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J. Chem. Phys. **142**, 184305 (2015); http://dx.doi.org/10.1063/1.4919690

Threshold photoelectron spectroscopy of unstable N-containing compounds: Resolution of ΔK subbands in $HNCO^+$ and vibrational resolution in NCO^+
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Two-dimensional spectra of electron collisions with acrylonitrile and methacrylonitrile reveal nuclear dynamics
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First-principles investigation of the dissociation and coupling of methane on small copper clusters: Interplay of collision dynamics and geometric and electronic effects
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Crossed-beam DC slice imaging of fluorine atom reactions with linear alkanes
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J. Chem. Phys. **142**, 184309 (2015); http://dx.doi.org/10.1063/1.4919099

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J. Chem. Phys. **142**, 184501 (2015); http://dx.doi.org/10.1063/1.4919947

Static dielectric properties of dense ionic fluids
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Satya N. Tripathy, Zaneta Wojnarowska, Justyna Knapik, Hideaki Shirota, Ranjit Biswas and Marian Paluch
J. Chem. Phys. **142**, 184504 (2015); http://dx.doi.org/10.1063/1.4919946

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J. Chem. Phys. **142**, 184505 (2015); http://dx.doi.org/10.1063/1.4920949

Surfaces, Interfaces, and Materials

Influence of grain size on optical properties of Sr_2CeO_4 nanocrystals
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An electron energy-loss study of picene and chrysene based charge transfer salts
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J. Chem. Phys. **142**, 184702 (2015); http://dx.doi.org/10.1063/1.4919881
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Stephen J. Cox, Shawn M. Kathmann, Ben Slater and Angelos Michaelides
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Molecular simulations of heterogeneous ice nucleation. II. Peeling back the layers
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Superpermittivity of nanoconfined water
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Liangbo Liang, Pan Zhu and Vincent Meunier
J. Chem. Phys. **142**, 184708 (2015); http://dx.doi.org/10.1063/1.4919682
Kinetically induced irreversibility in electro-oxidation and reduction of Pt surface
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J. Chem. Phys. **142**, 184709 (2015); http://dx.doi.org/10.1063/1.4920974

Polymers and Soft Matter

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J. Chem. Phys. **142**, 184902 (2015); http://dx.doi.org/10.1063/1.4919649
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J. Chem. Phys. **142**, 184904 (2015); http://dx.doi.org/10.1063/1.4920973
Ion mixing, hydration, and transport in aqueous ionic systems
Ying-Lung Steve Tse, Gregory A. Voth and Thomas A. Witten
J. Chem. Phys. **142**, 184905 (2015); http://dx.doi.org/10.1063/1.4921044

Biological Molecules and Networks

Dynamic memory of a single voltage-gated potassium ion channel: A stochastic nonequilibrium thermodynamic analysis
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J. Chem. Phys. **142**, 185101 (2015); http://dx.doi.org/10.1063/1.4920937
Designing pH induced fold switch in proteins
Anupaul Baruah and Parbati Biswas
J. Chem. Phys. **142**, 185102 (2015); http://dx.doi.org/10.1063/1.4920938

LETTERS TO THE EDITOR

Errata

Erratum: "Self-consistent embedding of density-matrix renormalization group wavefunctions in a density functional environment" [J. Chem. Phys. 142, 044111 (2015)]

Thomas Dresselhaus, Johannes Neugebauer, Stefan Knecht, Sebastian Keller, Yingjin Ma and Markus Reiher
J. Chem. Phys. **142**, 189901 (2015); http://dx.doi.org/10.1063/1.4921162

Publisher's Note: "Reactive scattering calculations for $^{87}Rb + {}^{87}RbHe \rightarrow Rb_2(^3\Sigma_u^+, v) + He$ ***from ultralow to intermediate energies" [J. Chem. Phys. 142, 164304 (2015)]***

Rocío Rodríguez-Cantano, Tomás González-Lezana, Rita Prosmiti, Gerardo Delgado-Barrio, Pablo Villarreal and Julius Jellinek
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