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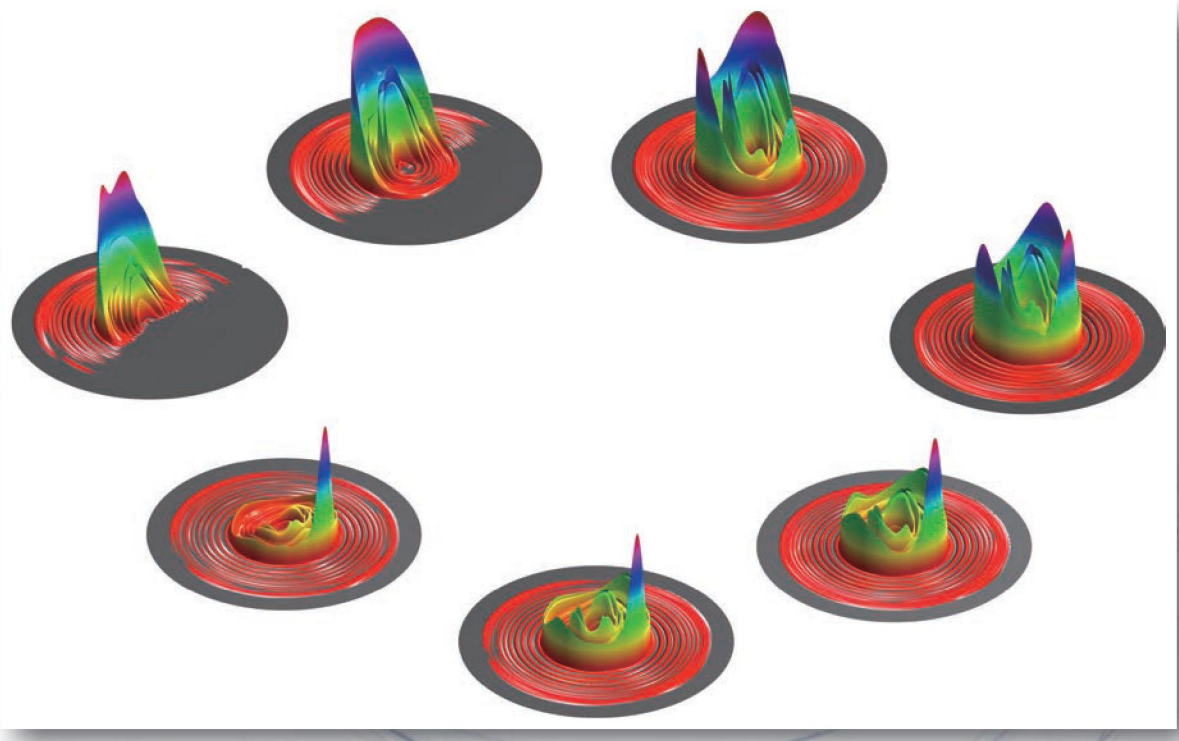

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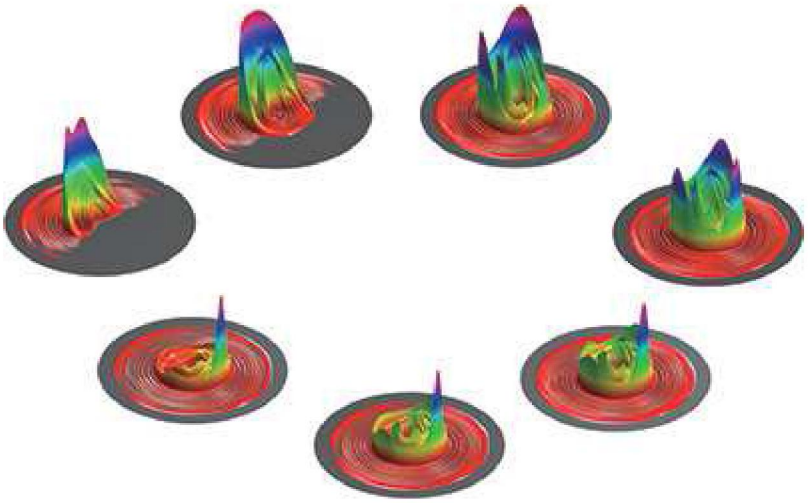

An accurate potential energy surface for the F + H_2 → HF + H reaction by the coupled-cluster method

COMMUNICATIONS

ARTICLES

Theoretical Methods and Algorithms

Stefan Medina, Jiajia Zhou, Zhen-Gang Wang and Friederike Schmid
J. Chem. Phys. **142**, 024103 (2015);

Restricted Hartree Fock using complex-valued orbitals: A long-known but neglected tool in electronic structure theory

David W. Small, Eric J. Sundstrom and Martin Head-Gordon
J. Chem. Phys. **142**, 024104 (2015);

Tensor decomposition techniques in the solution of vibrational coupled cluster response theory eigenvalue equations

Ian H. Godtliebsen, Mads Bøttger Hansen and Ove Christiansen
J. Chem. Phys. **142**, 024105 (2015);

Nudged-elastic band method with two climbing images: Finding transition states in complex energy landscapes

Nikolai A. Zarkevich and Duane D. Johnson
J. Chem. Phys. **142**, 024106 (2015);

A general non-Abelian density matrix renormalization group algorithm with application to the C_2 dimer

Sandeep Sharma
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Brownian dynamics simulations of coagulation of dilute uniform and anisotropic particles under shear flow spanning low to high Peclet numbers

Maziar Mohammadi, Eric D. Larson, Jun Liu and Ronald G. Larson
J. Chem. Phys. **142**, 024108 (2015);

The fast multipole method and point dipole moment polarizable force fields

Jonathan P. Coles and Michel Masella
J. Chem. Phys. **142**, 024109 (2015);

Thermal equilibrium properties of surface hopping with an implicit Langevin bath

M. C. Sherman and S. A. Corcelli
J. Chem. Phys. **142**, 024110 (2015);

On performance measures for infinite swapping Monte Carlo methods

J. D. Doll and Paul Dupuis
J. Chem. Phys. **142**, 024111 (2015);

Nonperturbative spin–boson and spin–spin dynamics and nonlinear Fano interferences: A unified dissipaton theory based study

Hou-Dao Zhang, Rui-Xue Xu, Xiao Zheng and YiJing Yan
J. Chem. Phys. 142, 024112 (2015);

An adaptive multi-level simulation algorithm for stochastic biological systems

C. Lester, C. A. Yates, M. B. Giles and R. E. Baker
J. Chem. Phys. **142**, 024113 (2015);

A pure-sampling quantum Monte Carlo algorithm

Egor Ospadov and Stuart M. Rothstein
J. Chem. Phys. **142**, 024114 (2015);

Stochastic Liouville equations for femtosecond stimulated Raman spectroscopy

Bijay Kumar Agarwalla, Hideo Ando, Konstantin E. Dorfman and Shaul Mukamel
J. Chem. Phys. **142**, 024115 (2015);

Atoms, Molecules, and Clusters

Theoretical study of thorium monoxide for the electron electric dipole moment search: Electronic properties of $H\,^3\Delta_1$ in ThO
L. V. Skripnikov and A. V. Titov
J. Chem. Phys. **142**, 024301 (2015);

New XDM-corrected potential energy surfaces for Ar–NO($X\,^2\Pi$): A comparison with CCSD(T) calculations and experiments
Michael Warehime, Erin R. Johnson and Jacek Kłos
J. Chem. Phys. **142**, 024302 (2015);

An accurate potential energy surface for the $F + H_2 \rightarrow HF + H$ reaction by the coupled-cluster method
Jun Chen, Zhigang Sun and Dong H. Zhang
J. Chem. Phys. **142**, 024303 (2015);

Low-temperature $D^+ + H_2$ reaction: A time-dependent coupled wave-packet study in hyperspherical coordinates
Tapas Sahoo, Sandip Ghosh, Satrajit Adhikari, Rahul Sharma and António J. C. Varandas
J. Chem. Phys. **142**, 024304 (2015);

Solvatochromism of 9,10-phenanthrenequinone: An electronic and resonance Raman spectroscopic study
Venkatraman Ravi Kumar, Nagappan Rajkumar and Siva Umapathy
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Unexpected methyl migrations of ethanol dimer under synchrotron VUV radiation
Weizhan Xiao, Yongjun Hu, Weixing Li, Jiwen Guan, Fuyi Liu, Xiaobin Shan and Liusi Sheng
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Optimal control of a Cope rearrangement by coupling the reaction path to a dissipative bath or a second active mode
Chenel, C. Meier, G. Dive and M. Desouter-Lecomte
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Near edge X-ray absorption mass spectrometry on coronene
G. Reitsma, L. Boschman, M. J. Deuzeman, S. Hoekstra, R. Hoekstra and T. Schlathölter
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Enhanced magnetism of Cu n clusters capped with N and endohedrally doped with Cr
Soumendu Datta, Radhashyam Banerjee and Abhijit Mookerjee
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Two-color two-photon excited fluorescence of indole: Determination of wavelength-dependent molecular parameters
Sebastian Herbrich, Tawfik Al-Hadhuri, Karl-Heinz Gericke, Peter S. Shternin, Andrey G. Smolin and Oleg S. Vasyutinskii

J. Chem. Phys. **142**, 024310 (2015);

Atom-diatom scattering dynamics of spinning molecules

C. J. Eyles, J. Floß, I. Sh. Averbukh and M. Leibscher

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Van der Waals coefficients beyond the classical shell model

Jianmin Tao, Yuan Fang, Pan Hao, G. E. Scuseria, Adrienn Ruzsinszky and John P. Perdew

J. Chem. Phys. **142**, 024312 (2015);

Probing the early stages of salt nucleation—Experimental and theoretical investigations of sodium/potassium thiocyanate cluster anions

S. H. M. Deng, Xiang-Yu Kong and Xue-Bin Wang

J. Chem. Phys. **142**, 024313 (2015);

Three-dimensional potential energy surface of Ar–CO

Yoshihiro Sumiyoshi and Yasuki Endo

J. Chem. Phys. **142**, 024314 (2015);

Direct observation of methyl rotor and vib-rotor states of S_0 toluene: A revised torsional barrier due to torsion-vibration coupling

Jason R. Gascooke, Edwina A. Virgo and Warren D. Lawrance

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The electronic states of TeH^+: A theoretical contribution

Levi Gonçalves dos Santos, Antonio Gustavo S. de Oliveira-Filho and Fernando R. Ornellas

J. Chem. Phys. **142**, 024316 (2015);

Accurate spectroscopy of polycyclic aromatic compounds: From the rotational spectrum of fluoren-9-one in the millimeter wave region to its infrared spectrum

Assimo Maris, Camilla Calabrese, Sonia Melandri and Susana Blanco

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Effect of Hartree-Fock exact exchange on intramolecular magnetic coupling constants of organic diradicals

Daeheum Cho, Kyoung Chul Ko, Yasuhiro Ikabata, Kazufumi Wakayama, Takeshi Yoshikawa, Hiromi Nakai and Jin Yong Lee

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Structural evolution of small ruthenium cluster anions

Eugen Waldt, Anna-Sophia Hehn, Reinhart Ahlrichs, Manfred M. Kappes and Detlef Schooss

J. Chem. Phys. **142**, 024319 (2015);

Liquids, Glasses, and Crystals

Multi-scale modelling of uranyl chloride solutions

Thanh-Nghi Nguyen, Magali Duvail, Arnaud Villard, John Jairo Molina, Philippe Guilbaud and Jean-François Dufrêche

J. Chem. Phys. **142**, 024501 (2015)

Water density fluctuations relevant to hydrophobic hydration are unaltered by attractions

Richard C. Remsing and Amish J. Patel

J. Chem. Phys. **142**, 024502 (2015);

Effect of the computational domain size and shape on the self-diffusion coefficient in a Lennard-Jones liquid

Gota Kikugawa, Shotaro Ando, Jo Suzuki, Yoichi Naruke, Takeo Nakano and Taku Ohara

J. Chem. Phys. **142**, 024503 (2015);

A first principles approach to the electronic properties of liquid and supercritical CO_2

Benedito J. Costa Cabral, Roberto Rivelino, Kaline Coutinho and Sylvio Canuto

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Flexible confinement leads to multiple relaxation regimes in glassy colloidal liquids

Ian Williams, Erdal C. Oğuz, Paul Bartlett, Hartmut Löwen and C. Patrick Royall

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Surfaces, Interfaces, and Materials

On the influence of polarization effects in predicting the interfacial structure and capacitance of graphene-like electrodes in ionic liquids

Eunsu Paek, Alexander J. Pak and Gyeong S. Hwang

J. Chem. Phys. **142**, 024701 (2015);

Structure and dynamics of H_2O vis-á-vis phenylalanine recognition at a DPPC lipid membrane via interfacial H-bond types: Insights from polarized FT-IRRAS and ADMP simulations

Nirod Kumar Sarangi, Nivarthi Ramesh and Archita Patnaik

J. Chem. Phys. **142**, 024702 (2015);

Experimental evidence for an optical interference model for vibrational sum frequency generation on multilayer organic thin film systems. I. Electric dipole approximation

Daniel B. O'Brien and Aaron M. Massari

J. Chem. Phys. **142**, 024703 (2015);

Experimental evidence for an optical interference model for vibrational sum frequency generation on multilayer organic thin film systems. II. Consideration for higher order terms

Daniel B. O'Brien and Aaron M. Massari

J. Chem. Phys. **142**, 024704 (2015);

Orbital line-up at poly[2-methoxy-5-(2'-ethylhexyloxy)-p-phenylene vinylene] (MEH-PPV)/poly(3-hexylthiophene) (P3HT) heterojunction

Wenfeng Wang and Rudy Schlaf

J. Chem. Phys. **142**, 024705 (2015);

Half-metallic properties, single-spin negative differential resistance, and large single-spin Seebeck effects induced by chemical doping in zigzag-edged graphene nanoribbons

Xi-Feng Yang, Wen-Qian Zhou, Xue-Kun Hong, Yu-Shen Liu, Xue-Feng Wang and Jin-Fu Feng

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Time-resolved x-ray diffraction and Raman studies of the phase transition mechanisms of methane hydrate

Hisako Hirai, Hirokazu Kadobayashi, Naohisa Hirao, Yasuo Ohishi, Michika Ohtake,Yoshitaka Yamamoto and Satoshi Nakano

J. Chem. Phys. **142**, 024707 (2015)

The nature of interfaces and charge trapping sites in photocatalytic mixed-phase $TiO_2$from first principles modeling

Polymers and Soft Matter

Biological Molecules and Networks

LETTERS TO THE EDITOR

Comments

Comment on "Steady-state fluctuations of a genetic feedback loop: An exact solution" [J. Chem. Phys. 137, 035104 (2012)]

Guilherme C. P. Innocentini, Alexandre F. Ramos and José Eduardo M. Hornos

J. Chem. Phys. **142**, 027101 (2015);