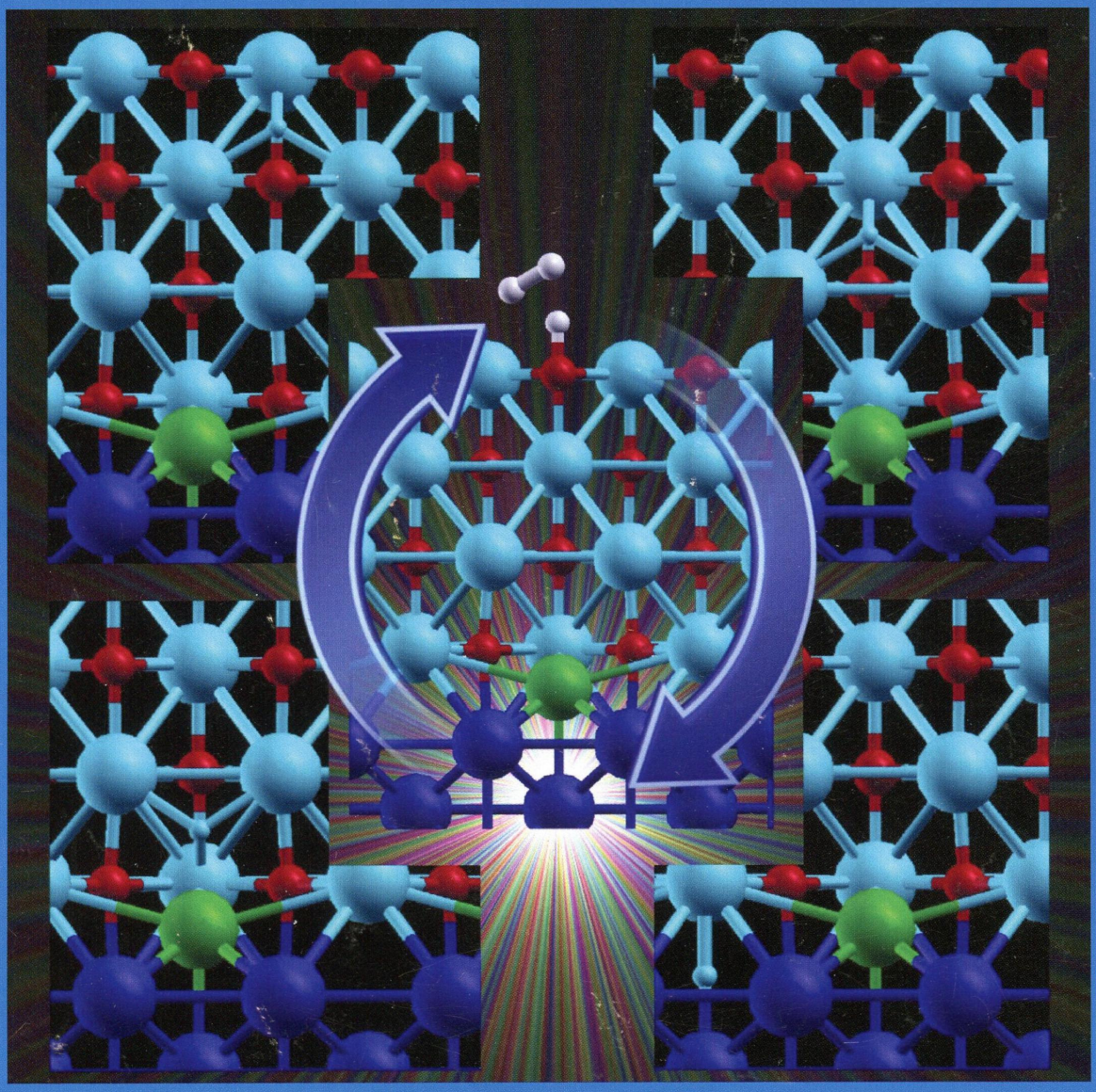
AUGUST 7, 2014
VOLUME 118
NUMBER 31
pubs.acs.org/JPCA

THE JOURNAL OF PHYSICAL CHEMISTRY A



ENERGETICS AND DYNAMICS OF MOLECULES, SOLIDS, AND SURFACES – QUITEL 2012

NiO-MgO/Mo(100) Interface from ab Initio Calculations Showing the Beginning of Hydrogen Permeation (see page 5A)

ISOLATED MOLECULES, CLUSTERS, RADICALS, AND IONS; ENVIRONMENTAL CHEMISTRY, GEOCHEMISTRY, AND ASTROCHEMISTRY; THEORY

ACS Publications
Most Trusted. Most Cited. Most Read.

www.acs.org

THE JOURNAL OF PHYSICAL CHEMISTRY A

AUGUST 7, 2014
VOLUME 118 ISSUE 31
JPCAFH 118(31) 5741−6132 (2014)
ISSN 1089-5639
Registered in the U.S. Patent and Trademark Office

ON THE COVER: Adsorption and permeation of atomic H on Ni-doped MgO oxide thin films is affected by the presence of a metallic support; H permeation through the unsupported NiO-MgO oxide is thermodynamically inhibited, but the presence of the metallic Mo makes permeation thermodynamically favored. Cover art by Daniel Torres Rangel. This special section was organized by Guest Editor Carlton A. Taft.

SPECIAL SECTION: ENERGETICS AND DYNAMICS OF MOLECULES, SOLIDS, AND SURFACES - QUITEL 2012

Guest Editor: Carlton A. Taft

Special Issue Preface

5741 dx.doi.org/10.1021/jp504188q

Energetics and Dynamics of Molecules, Solids, and Surfaces – QUITEL 2012
Carlton A. Taft*

Articles

5743 dx.doi.org/10.1021/jp403587s

Direct Evaluation of the Hyperconjugative Interactions in 1,1,1-Trihaloethane (CH_3CX_3, X = F, Cl, and Br)
Zhenhua Chen, Clémence Corminboeuf,* and Yirong Mo*

5748 dx.doi.org/10.1021/jp405877k

Adsorption of Pd, Pt, Cu, Ag, and Au Monomers on NiAl(110) Surface: A Comparative Study from DFT Calculations
Miguel A. San-Miguel, Edgard P. M. Amorim, and E. Z. da Silva*

5756 dx.doi.org/10.1021/jp408872x

Theoretical Study of Hydrogen Permeation through Mixed NiO–MgO Films Supported on Mo(100): Role of the Oxide–Metal Interface
Daniel Torres, Francesc Illas,* and Ping Liu

5762 dx.doi.org/10.1021/jp4099045

Potential Energy Surfaces of WC_6 Clusters in Different Spin States
C. Z. Hadad,* Elizabeth Florez, Gabriel Merino, José Luis Cabellos, Franklin Ferraro, and Albeiro Restrepo*

5769 dx.doi.org/10.1021/jp410564p
Potentiated Electron Transference in α-Ag_2WO_4 Microcrystals with Ag Nanofilaments as Microbial Agent
Valéria M. Longo,* Camila C. De Foggi, Mateus M. Ferrer, Amanda F. Gouveia, Rafaela S. André, Waldir Avansi, Carlos E. Vergani, Ana L Machado, Juan Andrés, Laécio S. Cavalcante, Antonio C. Hernandes, and Elson Longo

5779 dx.doi.org/10.1021/jp410754a
Periodic Quantum Chemical Studies on Anhydrous and Hydrated Acid Clinoptilolite
Karell Valdiviés Cruz, Anabel Lam, and Claudio M. Zicovich-Wilson*

5790 dx.doi.org/10.1021/jp410810q
Isomerization of Δ^5-Androstene-3,17-dione into Δ^4-Androstene-3,17-dione Catalyzed by Human Glutathione Transferase A3-3: A Computational Study Identifies a Dual Role for Glutathione
Daniel F. A. R. Dourado, Pedro Alexandrino Fernandes, Bengt Mannervik, and Maria João Ramos*

5801 dx.doi.org/10.1021/jp411173k
Silica-Based Materials as Drug Adsorbents: First Principle Investigation on the Role of Water Microsolvation on Ibuprofen Adsorption
Massimo Delle Piane, Stefano Vaccari, Marta Corno, and Piero Ugliengo*

5808 dx.doi.org/10.1021/jp411230w
Hydrophobic Noncovalent Interactions of Inosine-Phenylalanine: A Theoretical Model for Investigating the Molecular Recognition of Nucleobases
Lucas A. Santos, Elaine F. F. da Cunha, Matheus P. Freitas, and Teodorico C. Ramalho*

5818 dx.doi.org/10.1021/jp4114283
Relativistic Four-Component Potential Energy Curves for the Lowest 23 Covalent States of Molecular Bromine (Br_2)
José da Silva Gomes, Ricardo Gargano, João B. L. Martins, and Luiz Guilherme M. de Macedo*

5823 dx.doi.org/10.1021/jp4114706
First-Principles Calculations and Electron Density Topological Analysis of Covellite (CuS)
A. Morales-García, Antonio Lenito Soares Jr., Egon C. Dos Santos, Heitor A. de Abreu, and Hélio A. Duarte*

5832 dx.doi.org/10.1021/jp411500j
Density Functional Theory Study of the Water Dissociation on Platinum Surfaces: General Trends
José L. C. Fajín,* M. Natália D. S. Cordeiro, and José R. B. Gomes*

5841 dx.doi.org/10.1021/jp411577a
Magnetic Exchange Couplings from Noncollinear Perturbation Theory: Dinuclear Cu^{II} Complexes
Jordan J. Phillips and Juan E. Peralta*

5848 dx.doi.org/10.1021/jp411662c
Fusion of Ligand-Coated Nanoparticles with Lipid Bilayers: Effect of Ligand Flexibility
Reid C. Van Lehn and Alfredo Alexander-Katz*

5857 dx.doi.org/10.1021/jp411764t
Preparation of TiO_2/SnO_2 Thin Films by Sol–Gel Method and Periodic B3LYP Simulations
Emerson A. Floriano, Luis V. A. Scalvi, Margarida J. Saeki, and Julio R. Sambrano*

5866 dx.doi.org/10.1021/jp4118198
B3LYP Periodic Study of the Physicochemical Properties of the Nonpolar (010) Mg-Pure and Fe-Containing Olivine Surfaces
Javier Navarro-Ruiz, Piero Ugliengo, Albert Rimola,* and Mariona Sodupe*

5876 dx.doi.org/10.1021/jp4120892
Singly Occupied MOs in Mono- and Diradical Conjugated Hydrocarbons: Comparison between Variational Single-Reference, π-Fully Correlated and Hückel Descriptions
Nicolas Suaud, Renaud Ruamps, Jean-Paul Malrieu, and Nathalie Guihéry*

5885 dx.doi.org/10.1021/jp501058x
DFT/TDDFT Study of the Adsorption of N3 and N719 Dyes on ZnO(10$\bar{1}$0) Surfaces
Jon M. Azpiroz and Filippo De Angelis*

5894 dx.doi.org/10.1021/jp503558s
Gold–Bismuth Clusters
Ana Martínez*

Articles

Kinetics and Dynamics

5903 dx.doi.org/10.1021/jp504018k
S-Oxygenation of Thiocarbamides V: Oxidation of Tetramethylthiourea by Chlorite in Slightly Acidic Media
Tabitha Chigwada, Wilbes Mbiya, Kudzanai Chipiso, and Reuben H. Simoyi*

5915 dx.doi.org/10.1021/jp504757g
Time-Dependent Quantum Wave Packet Dynamics of S + OH Reaction on Its Electronic Ground State
Sugata Goswami, T. Rajagopala Rao, S. Mahapatra,* B. Bussery-Honvault, and P. Honvault

5927 dx.doi.org/10.1021/jp505145j
Thermal Decomposition of Propargyl Alcohol: Single Pulse Shock Tube Experimental and ab Initio Theoretical Study
N. Sharath, K. P. J. Reddy, and E. Arunan*

Spectroscopy, Photochemistry, and Excited States

5939 S dx.doi.org/10.1021/jp5039688

UV Photochemistry of Peroxyformic Acid (HC(O)OOH): An Experimental and Computational Study Investigating 355 nm Photolysis
Yogesh N. Indulkar, Matthew K. Louie, and Amitabha Sinha*

5950 S dx.doi.org/10.1021/jp412564u

Electronic Properties of $FC(O)SCH_2CH_3$. A Combined Helium(I) Photoelectron Spectroscopy and Synchrotron Radiation Study
Lucas S. Rodríguez Pirani, Mauricio F. Erben,* Mariana Geronés, Rosana M. Romano, Reinaldo L. Cavasso Filho, Chunping Ma, Maofa Ge, and Carlos O. Della Védova*

5961 dx.doi.org/10.1021/jp504391s

Ultrafast Excited State Dynamics in 9,9′-Bifluorenylidene
Jamie Conyard, Ismael A. Heisler, Wesley R. Browne, Ben L. Feringa, Saeed Amirjalayer,* Wybren Jan Buma, Sander Woutersen, and Stephen R. Meech*

5969 S dx.doi.org/10.1021/jp504935g

Intermolecular Stabilization of 3,3′-Diamino-4,4′-azoxyfurazan (DAAF) Compressed to 20 GPa
Raja S. Chellappa,* Dana M. Dattelbaum,* Joshua D. Coe, Nenad Velisavljevic, Lewis L. Stevens, and Zhenxian Liu

5983 dx.doi.org/10.1021/jp505255a

Role of Photophysics Processes in Thermal Lens Spectroscopy of Fluids: A Theoretical Study
L. C. Malacarne, E. L. Savi, M. L. Baesso, E. K. Lenzi, and N. G. C. Astrath*

5989 S dx.doi.org/10.1021/jp505308v

A Preorganized Hydrogen Bond Network and Its Effect on Anion Stability
Masoud Samet, Xue-Bin Wang,* and Steven R. Kass*

5994 S dx.doi.org/10.1021/jp505335c

Molecular Structure, Infrared Spectra, Photochemistry, and Thermal Properties of 1-Methylhydantoin
Bernardo A. Nogueira, Gulce O. Ildiz, João Canotilho, M. Ermelinda S. Eusébio, and Rui Fausto*

6009 S dx.doi.org/10.1021/jp505740j

Infrared Spectra and Structures of the Neutral and Charged $CrCO_2$ and $Cr(CO_2)_2$ Isomers in Solid Neon
Qingnan Zhang, Mohua Chen, and Mingfei Zhou*

6018 S dx.doi.org/10.1021/jp505752c

Efficient Amplitude-Modulated Pulses for Triple- to Single-Quantum Coherence Conversion in MQMAS NMR
Henri Colaux, Daniel M. Dawson, and Sharon E. Ashbrook*

6026 dx.doi.org/10.1021/jp5060588
High-Contrast Electroswitching of Emission and Coloration Based on Single-Molecular Fluoran Derivatives
Kenji Kanazawa, Kazuki Nakamura,* and Norihisa Kobayashi*

Environmental and Atmospheric Chemistry, Aerosol Processes, Geochemistry, and Astrochemistry

6034 dx.doi.org/10.1021/jp5032306
Experimental Studies of $H^{13}CO^+$ Recombining with Electrons at Energies between 2−50 000 meV
Mathias Hamberg, Iryna Kashperka, Richard D. Thomas, Evelyne Roueff, Vitali Zhaunerchyk, Mathias Danielsson, Magnus af Ugglas, Fabian Österdahl, Erik Vigren, Magdalena Kaminska, Anders Källberg, Ansgar Simonsson, Andras Paal, Maryvonne Gerin, Mats Larsson, and Wolf D. Geppert*

Molecular Structure, Quantum Chemistry, and General Theory

6050 dx.doi.org/10.1021/jp5058989
A Semi-homodesmotic Approach for Estimating Ring Strain Energies (RSEs) of Highly Substituted Cyclopropanes That Minimizes Use of Acyclic References and Cancels Steric Interactions: RSEs for *c*-C_3R_6 that Make Sense
Ashley M. De Lio, Bridget L. Durfey, Austin L. Gille, and Thomas M. Gilbert*

6060 dx.doi.org/10.1021/jp5058995
Application of a Semi-homodesmotic Approach in Estimating Ring Strain Energies (RSEs) of Highly Substituted Cyclobutanes: RSEs for *c*-C_4R_8 That Make Sense
Thomas M. Gilbert*

6068 dx.doi.org/10.1021/jp411810y
Polymorphism in Paracetamol: Evidence of Additional Forms IV and V at High Pressure
Spencer J. Smith, Matthew M. Bishop, Jeffrey M. Montgomery, Tracy P. Hamilton, and Yogesh K. Vohra*

6078 dx.doi.org/10.1021/jp5018339
From Thiol to Sulfonic Acid: Modeling the Oxidation Pathway of Protein Thiols by Hydrogen Peroxide
Laura A. H. van Bergen, Goedele Roos, and Frank De Proft*

6085 dx.doi.org/10.1021/jp503900m
Modulating the Electronic Structure of Chromophores by Chemical Substituents for Efficient Energy Transfer: Application to Fluorone
Andrew M. Sand, Claire Liu, Andrew J. S. Valentine, and David A. Mazziotti*

6092 dx.doi.org/10.1021/jp504172g
Oxygen Atom Transfer Reactions from Mimoun Complexes to Sulfides and Sulfoxides. A Bonding Evolution Theory Analysis
Patricio González-Navarrete,* Fabricio R. Sensato, Juan Andrés,* and Elson Longo

6104 dx.doi.org/10.1021/jp504408u

All-Carbon, Neutral Analogue of ExBox^{4+}: A DFT Study of Polycyclic Aromatic Hydrocarbon Binding
Steven M. Bachrach* and Ann E. Andrews

6112 dx.doi.org/10.1021/jp5058463

Interaction of Anions with Substituted Buckybowls. The Anion's Nature and Solvent Effects
Alba Campo-Cacharrón, Enrique M. Cabaleiro-Lago,* Iván González-Veloso, and Jesús Rodríguez-Otero

6125 dx.doi.org/10.1021/jp505276n

Vertical Ionization Energies of Free Radicals and Electron Detachment Energies of Their Anions: A Comparison of Direct and Indirect Methods Versus Experiment
Adriana Pérez-González, Annia Galano,* and J. V. Ortiz*

Supporting Information available via online article