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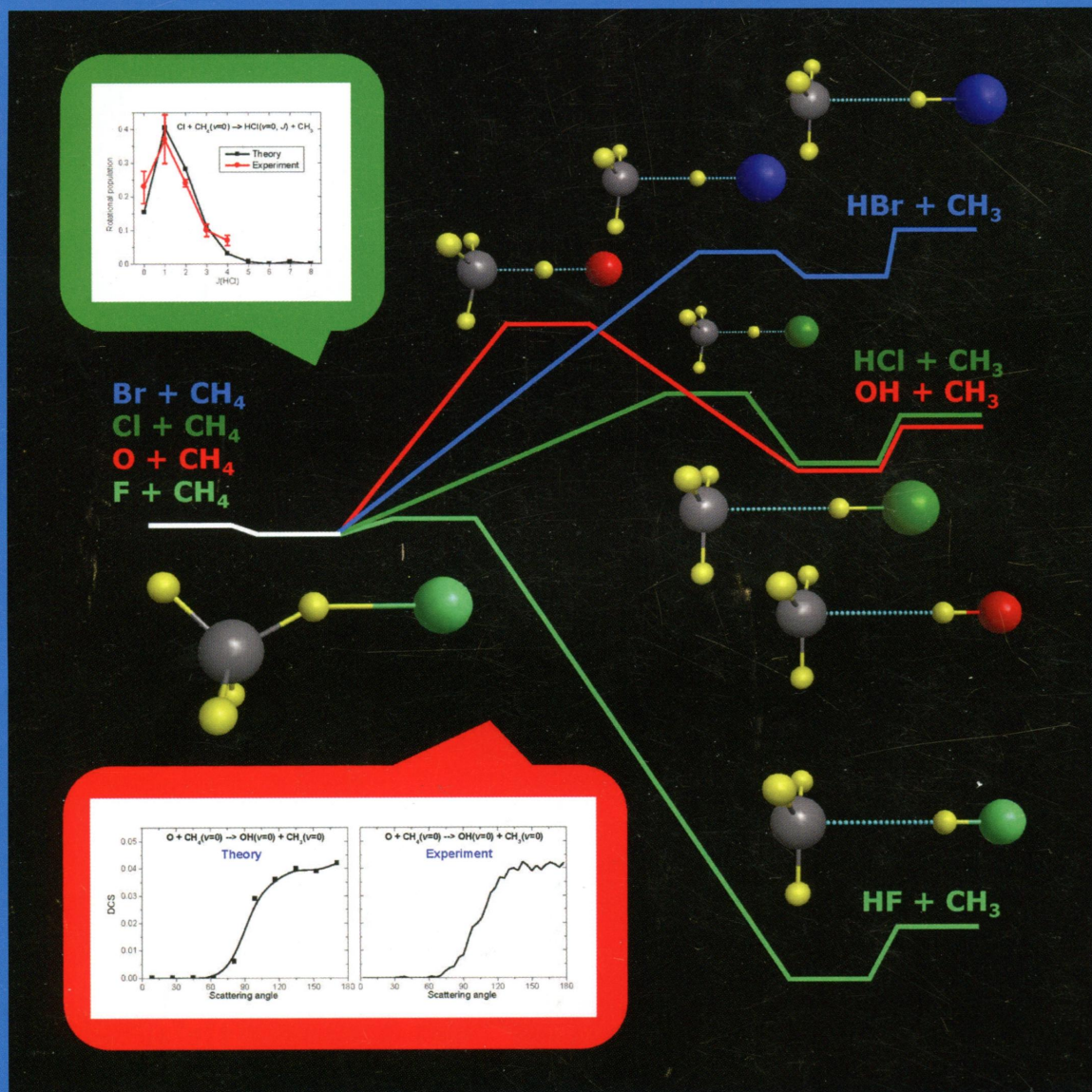
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A



Schematic of the Energies of Indicated X + CH₄ Reactions from *ab Initio* Potential Surfaces (see page 5A)

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



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ON THE COVER: Schematic of the energies of Br, Cl, O, and F + CH₄ reactions from high-level, *ab initio* permutationally invariant potential surfaces used in dynamics calculations. Top left graph from Czakó, G.; Bowman, J. M. Dynamics of the Reaction of Methane with Chlorine Atom on an Accurate Potential Energy Surface. *Science* **2011**, *334*, 343–346. Reprinted with permission from AAAS. Bottom left graphs adapted from Czakó, G.; Liu, R.; Yang, M.; Bowman, J. M.; Guo, H. Quasiclassical Trajectory Studies of the O(³P) + CX₄(*v*_k = 0, 1) → OX(*v*) + CX₃(*n*₁*n*₂*n*₃*n*₄) [X = H and D] Reactions on an *ab Initio* Potential Energy Surface. *J. Phys. Chem. A* **2013**, *117*, 6409–6420. See page 2839.


Feature Article

2839 dx.doi.org/10.1021/jp500085h
Reaction Dynamics of Methane with F, O, Cl, and Br on *ab Initio* Potential Energy Surfaces
Gábor Czakó* and Joel M. Bowman*

Articles


Kinetics and Dynamics

2865  dx.doi.org/10.1021/jp410704b
PAH Growth Initiated by Propargyl Addition: Mechanism Development and Computational Kinetics
Abhijeet Raj, Mariam J. Al Rashidi,* Suk Ho Chung, and S. Mani Sarathy

2886  dx.doi.org/10.1021/jp412299p
Effects of CF₃ and CH₃ Groups on the Threshold Energy for the Unimolecular Interchange Reaction of Cl⁻ and F-Atoms in CF₃CHFCH₂Cl and CH₃CHFCH₂Cl
Corey E. McClintock, Kylie C. Smith, George L. Heard, D. W. Setser, and Bert E. Holmes*

2897 dx.doi.org/10.1021/jp501455z
Nitrogen Oxides As a Chemistry Trap in Detonating Oxygen-Rich Materials
Nir Goldman* and Sorin Bastea

Spectroscopy, Photochemistry, and Excited States


2904  dx.doi.org/10.1021/jp4090266
Density Functional Theoretical Modeling, Electrostatic Surface Potential and Surface Enhanced Raman Spectroscopic Studies on Biosynthesized Silver Nanoparticles: Observation of 400 pM Sensitivity to Explosives
Sanchita Sil, Deepika Chaturvedi, Keerthi B. Krishnappa, Srividya Kumar, S. N. Asthana, and Siva Umaphathy*

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[dx.doi.org/10.1021/jp412482p](https://doi.org/10.1021/jp412482p)

Electronic Spectroscopy of 1-(Phenylethynyl)naphthalene

Philipp Constantinidis, Melanie Lang, Jörg Herterich, Ingo Fischer,* Johannes Auerswald, and Anke Krueger

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[dx.doi.org/10.1021/jp412804d](https://doi.org/10.1021/jp412804d)

Comparative Study on the Properties of Hydration Water of Na- and K-Halide Ions by Raman OH/OD-stretching Spectroscopy and Dielectric Relaxation Data

Yuichiro Okazaki, Tetsuo Taniuchi, George Mogami, Nobuyuki Matubayasi, and Makoto Suzuki*

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[dx.doi.org/10.1021/jp501906u](https://doi.org/10.1021/jp501906u)

Circular Dichroism Spectra of Uridine Derivatives: ChiraSac Study

Tomoo Miyahara, Hiroshi Nakatsuji,* and Takehiko Wada


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[dx.doi.org/10.1021/jp502465j](https://doi.org/10.1021/jp502465j)

Cavity-Enhanced Overtone Spectroscopy of Methanol in Aprotic Solvents: Probing Solute–Solvent Interactions and Self-Associative Behavior

Da-Sol Kuen and Karl J. Feierabend*

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

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[dx.doi.org/10.1021/jp412404w](https://doi.org/10.1021/jp412404w)

Enhanced Removal of Uranium(VI) by Nanoscale Zerovalent Iron Supported on Na–Bentonite and an Investigation of Mechanism

Gudong Sheng, Xiaoyu Shao, Yimin Li,* Jianfa Li, Huaping Dong, Wei Cheng, Xing Gao, and Yuying Huang

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[dx.doi.org/10.1021/jp412654s](https://doi.org/10.1021/jp412654s)

Mercury Oxidation via Chlorine, Bromine, and Iodine under Atmospheric Conditions: Thermochemistry and Kinetics

Itsaso Auzmendi-Murua, Álvaro Castillo, and Joseph W. Bozzelli*

Molecular Structure, Quantum Chemistry, and General Theory

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[dx.doi.org/10.1021/jp500191v](https://doi.org/10.1021/jp500191v)

Structural and Electronic Properties of $TM_n[(BN)_3H_6]_m$ Complexes with $TM = Co$ ($n, m = 1–3$) and with $TM = Fe, Ni, Ru, Rh, Pd$ ($n = m = 1–3$)

F. Aguilera-Granja, R. H. Aguilera-del-Toro, A. Vega, and L. C. Balbás*

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[dx.doi.org/10.1021/jp500447m](https://doi.org/10.1021/jp500447m)

Impact of Lewis Base on Chemical Reactivity and Separation Efficiency for Hydrated Fourth-Row Transition Metal (II) Complexes: An ONIOM DFT/MM Study

Dingsheng He* and Ming Ma

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[dx.doi.org/10.1021/jp501064c](https://doi.org/10.1021/jp501064c)

Scalar Relaxation of the Second Kind. A Potential Source of Information on the Dynamics of Molecular Movements. 3. A ^{13}C Nuclear Spin Relaxation Study of CBrX_3 ($X = \text{Cl}, \text{CH}_3, \text{Br}$) Molecules

Dominika Kubica, Artur Wodyński, Anna Kraska-Dziadecka, and Adam Gryff-Keller*

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[dx.doi.org/10.1021/jp5010677](https://doi.org/10.1021/jp5010677)

Does the Preferred Mechanism of a Catalytic Transformation Depend on the Density Functional? Ethylene Hydrosilylation by a Metal Complex as a Case Study

Yin Wu, Alexander Genest, and Notker Rösch*

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[dx.doi.org/10.1021/jp5017032](https://doi.org/10.1021/jp5017032)

Aromatic Character of Nanographene Model Compounds

Kenkichi Sakamoto, Naoko Nishina, Toshiaki Enoki, and Jun-ichi Aihara*

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[dx.doi.org/10.1021/jp5021406](https://doi.org/10.1021/jp5021406)

Theoretical Study of Water Cluster Catalyzed Decomposition of Formic Acid

Satoshi Inaba*