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SEPTEMBER 11, 2014

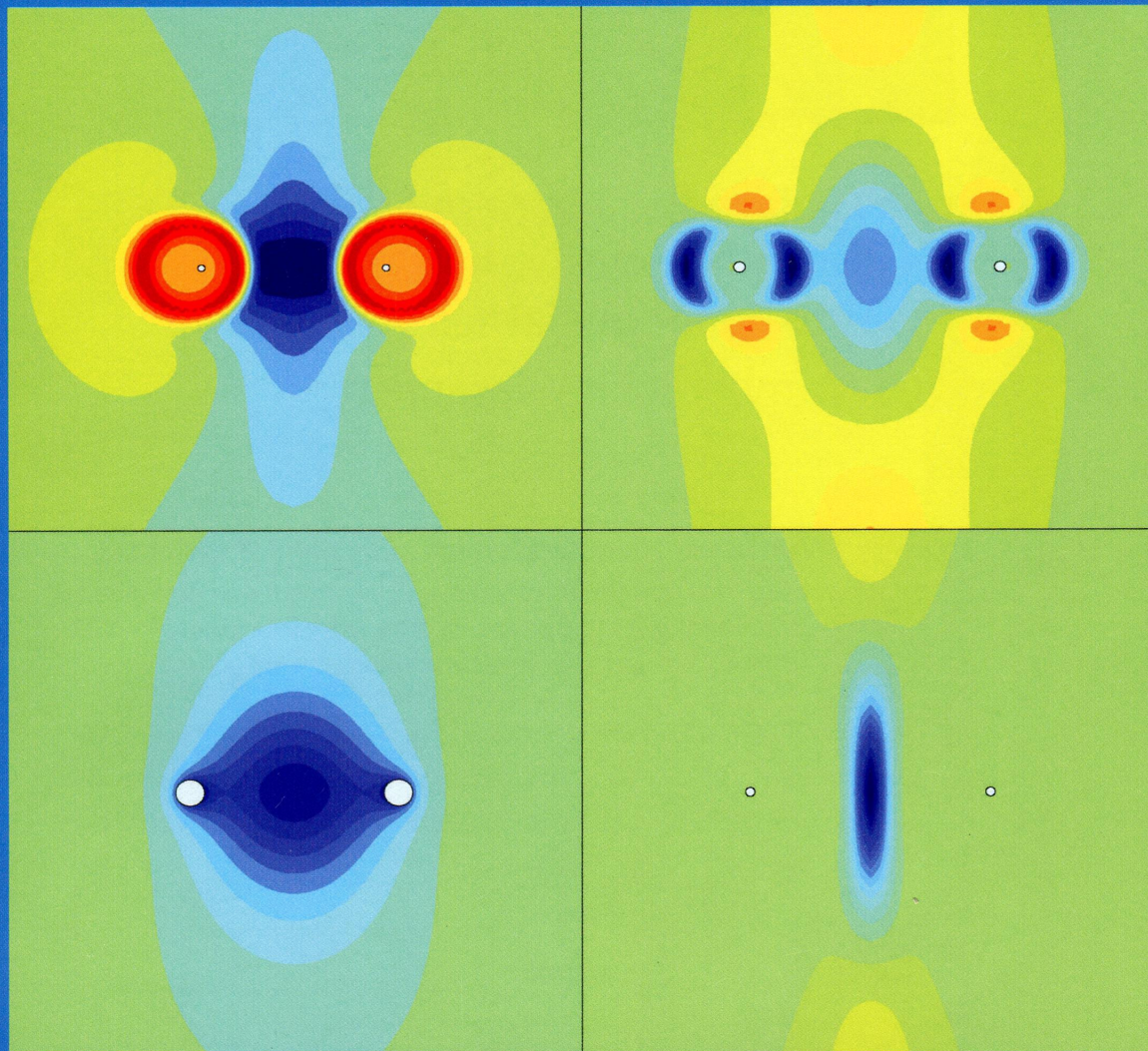
VOLUME 118

NUMBER 36

pubs.acs.org/JPCA

THE JOURNAL OF  
PHYSICAL  
CHEMISTRY

A



Partition Potentials  
for the First Four  
Homonuclear  
Diatomic. Clockwise  
from Top Left: Li<sub>2</sub>, Be<sub>2</sub>,  
He<sub>2</sub>, H<sub>2</sub>  
(see page 5A)

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



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**ON THE COVER:** The cover displays plots of partition potentials for the first four homonuclear diatomic molecules. Clockwise from top left:  $\text{Li}_2$ ,  $\text{Be}_2$ ,  $\text{He}_2$ ,  $\text{H}_2$ . The partition potential is a molecular fingerprint provided by partition density-functional theory (PDFT). It is the global one-body external potential that, when added to each of the nuclear potentials of the isolated fragments, deforms their electronic densities so that their sum is exactly the molecular density obtained from a Kohn–Sham (KS) calculation (the local density approximation was used for the potentials shown here). See page 7623.

## Feature Article

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[dx.doi.org/10.1021/jp504058s](https://doi.org/10.1021/jp504058s)**Density-Based Partitioning Methods for Ground-State Molecular Calculations**

Jonathan Nafziger and Adam Wasserman\*

## Articles

### Kinetics and Dynamics

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[dx.doi.org/10.1021/jp502470j](https://doi.org/10.1021/jp502470j)**Reactions of Atomic Hydrogen with Formic Acid and Carbon Monoxide in Solid Parahydrogen I: Anomalous Effect of Temperature**

Leif O. Paulson, Fredrick M. Mutunga, Shelby E. Follett, and David T. Anderson\*

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[dx.doi.org/10.1021/jp502469p](https://doi.org/10.1021/jp502469p)**Reactions of Atomic Hydrogen with Formic Acid and Carbon Monoxide in Solid Parahydrogen II: Deuterated Reaction Studies**

William R. Wonderly and David T. Anderson\*

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[dx.doi.org/10.1021/jp506140m](https://doi.org/10.1021/jp506140m)**Effect of Hydration on the Kinetics of Proton-Bound Dimer Formation: Experimental and Theoretical Study**

Younes Valadbeigi,\* Hossein Farrokhpour,\* and Mahmoud Tabrizchi\*

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[dx.doi.org/10.1021/jp504722q](https://doi.org/10.1021/jp504722q)**Graph Theoretical Analysis on the Kinetic Rate Equations of Linear Chain and Cyclic Reaction Networks**

Somnath Karmakar and Bholanath Mandal\*

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[dx.doi.org/10.1021/jp5066067](https://doi.org/10.1021/jp5066067)

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