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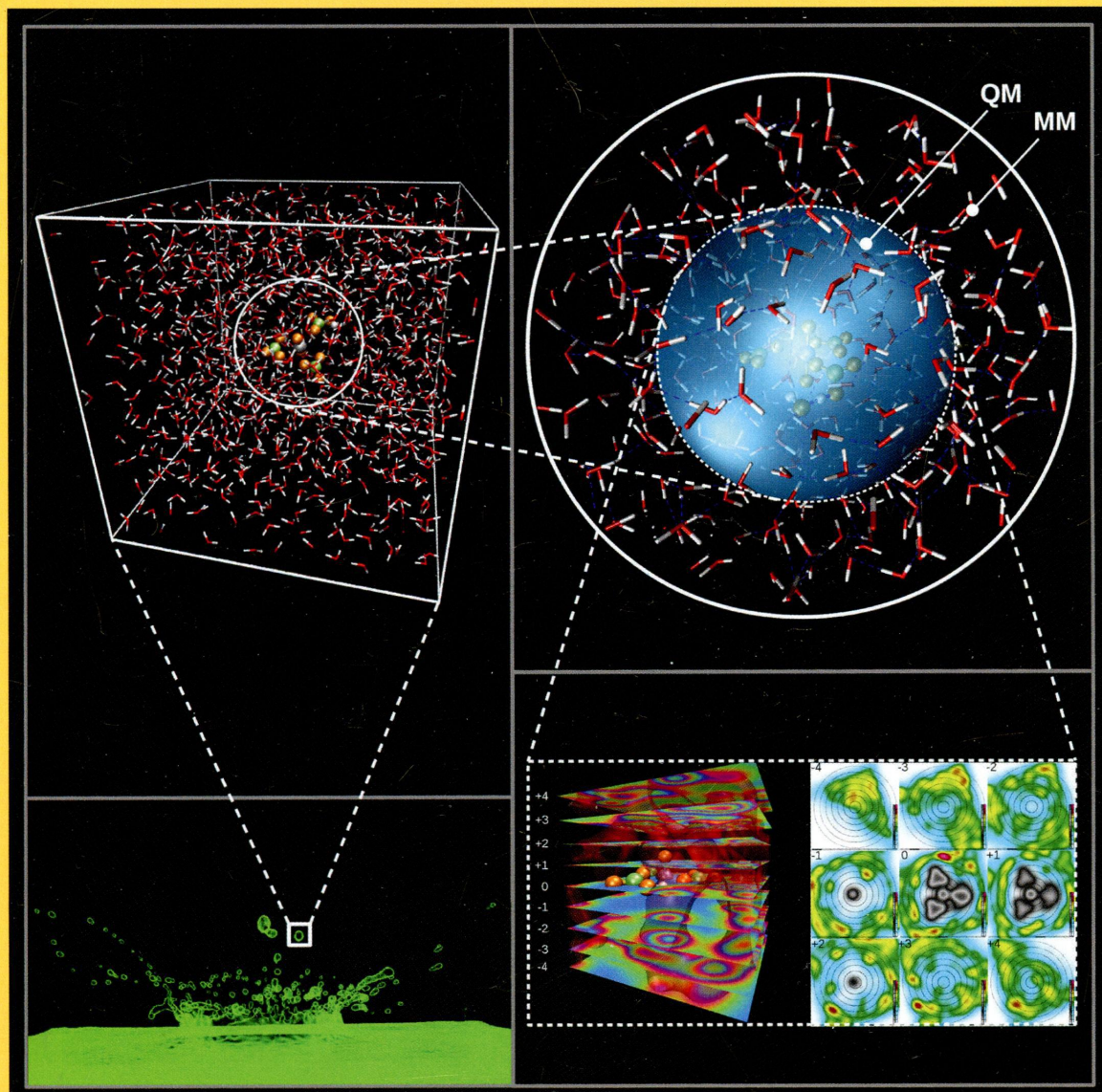
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B

Characterization
of Structural and
Dynamical Properties
of $[\text{UO}_2(\text{CO}_3)_2\text{HCO}_3]^{3-}$
via Hybrid QM/MM
MD Simulations
(see page 12938)



BIOPHYSICAL CHEMISTRY, BIOMATERIALS, LIQUIDS, AND SOFT MATTER



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ON THE COVER: Molecular dynamics (MD) simulations are a versatile tool to investigate structural and dynamical properties of chemical systems on a microscopic scale. The performance of such simulations strongly depends on the applied level of theory to achieve an accurate description of the potential energy and the associated interatomic forces. Hybrid QM/MM simulations are especially suitable for the investigation of chemical systems, since they combine the high accuracy of quantum mechanical (QM) methods, applied to the chemically most relevant part, with the efficiency of molecular mechanical (MM) techniques, which are assumed sufficiently accurate to describe the remaining part of the system. This approach proved particularly suitable for the treatment of coordination complexes such as the highly charged $[\text{UO}_2(\text{CO}_3)_2\text{HCO}_3]^{3-}$ system investigated in this study. A detailed analysis of the structural and dynamical properties of this environmentally highly relevant species based on QM/MM MD simulation data is discussed in the presented work. [Figures have been created with Blender (<http://www.blender.org/>) and VMD (Humphrey, W.; Dalke, A.; Schulten, K. VMD: Visual Molecular Dynamics. *J. Mol. Graphics*, 1996, 14, 33–38. <http://www.ks.uiuc.edu/Research/vmd/>.)] Cover art created by Andreas O. Tirlir. See page 12938.

Review Article

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DOI: 10.1021/jp5059885

Wanted: Scalable Tracers for Diffusion Measurements

Michael J. Saxton*

Articles

Biophysical Chemistry and Biomolecules

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DOI: 10.1021/jp507971v

Underlying Thermodynamics of pH-Dependent Allostery

Natali V. Di Russo, Marcelo A. Marti, and Adrian E. Roitberg*

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DOI: 10.1021/jp508360k

Kinetics Study on the HIV-1 Ectodomain Protein Quaternary Structure Formation Reveals Coupling of Chain Folding and Self-Assembly in the Refolding Cascade

Shu-Fang Cheng, Tai-Ching Sung, Chung-Chieh Chang, Mei-Ju Chou, Yun-Wei Chiang, and Ding-Kwo Chang*

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DOI: 10.1021/jp508547y

Terahertz Chiroptical Spectroscopy of an α -Helical Polypeptide: A Molecular Dynamics Simulation Study

Jun-Ho Choi and Minhaeng Cho*

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DOI: 10.1021/jp508632h

Infinitely Dilute Partial Molar Properties of Proteins from Computer Simulation

Elizabeth A. Ploetz and Paul E. Smith*

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DOI: 10.1021/jp509053q

Identification and Relative Quantification of Tyrosine Nitration in a Model Peptide Using Two-Dimensional Infrared Spectroscopy

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DOI: 10.1021/jp5101413

Internal vs Fishhook Hairpin DNA: Unzipping Locations and Mechanisms in the α -Hemolysin Nanopore

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Biomaterials, Surfactants, and Membranes

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DOI: 10.1021/jp504427a

Exploring the Local Elastic Properties of Bilayer Membranes Using Molecular Dynamics Simulations

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Validity of Linear Response Theory for Time-Dependent Fluorescence in *Staphylococcus* Nuclease
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Field- and Temperature-Dependent ^{13}C NMR Studies of the EDTA– Zn^{2+} Complex: Insight into Structure and Dynamics via Relaxation Measurements
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Unraveling the Mechanism of a Reversible Photoactivated Molecular Proton Crane
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Determination of the Enthalpy of Vaporization and Prediction of Surface Tension for Ionic Liquid 1-Alkyl-3-methylimidazolium Propionate $[\text{C}_n\text{mim}][\text{Pro}]$ ($n = 4, 5, 6$)
Jing Tong,* Hong-Xu Yang, Ru-Jing Liu, Chi Li, Li-Xin Xia,* and Jia-Zhen Yang

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DOI: 10.1021/jp5092784

Solvation and Rotation Dynamics in the Trihexyl(tetradecyl)phosphonium Chloride Ionic Liquid/Methanol Cosolvent System
Kathleen M. Barra, Randy P. Sabatini, Zachery P. McAtee, and Mark P. Heitz*

Glasses, Colloids, Polymers, and Soft Matter

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DOI: 10.1021/jp5060843

Doping of Polyaniline with 6-Cyano-2-naphthol
Debasree Das, Anindya Datta,* and Aliasgar Q. Contractor*

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DOI: 10.1021/jp5072082

Volume Fraction of Ether Is a Significant Factor in Controlling Conductivity in Proton Conducting Polyether Based Polymer Sol–Gel Electrolytes
Benjamin Yancey, Jonathan Jones, and Jason E. Ritchie*

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DOI: 10.1021/jp509175a

Small Angle Neutron Scattering Study of Complex Coacervate Micelles and Hydrogels Formed from Ionic Diblock and Triblock Copolymers

Daniel V. Krogstad, Soo-Hyung Choi, Nathaniel A. Lynd, Debra J. Audus, Sarah L. Perry, Jeffrey D. Gopez, Craig J. Hawker, Edward J. Kramer, and Matthew V. Tirrell*

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DOI: 10.1021/jp5093702

Crystallization, Recrystallization, and Melting Lines in Syndiotactic Polypropylene Crystallized from Quiescent Melt and Semicrystalline State Due to Stress-Induced Localized Melting and Recrystallization

Ying Lu, Yaotao Wang, Lianlian Fu, Zhiyong Jiang, and Yongfeng Men*