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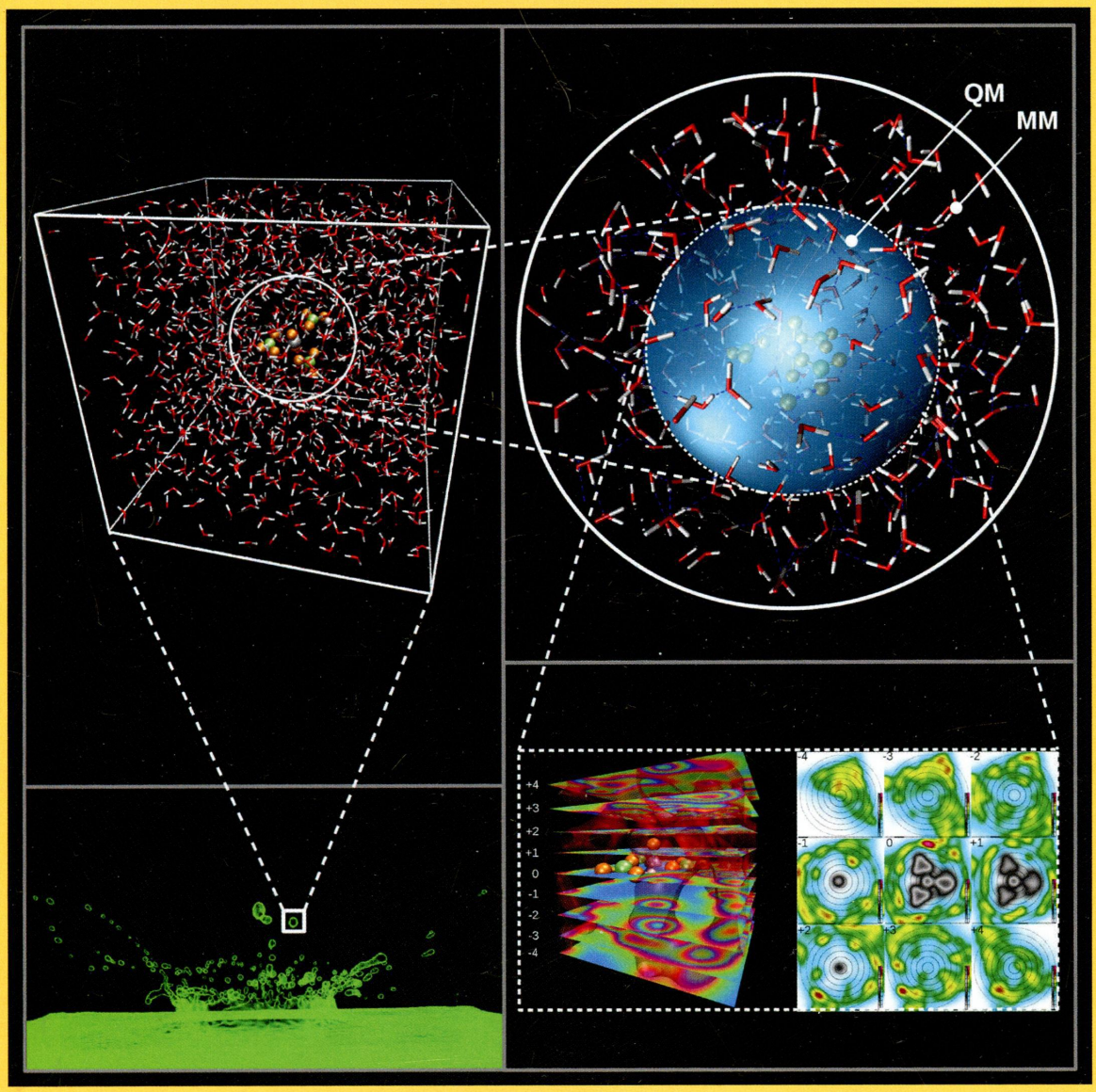

Characterization of Structural and Dynamical Properties of $[UO_2(CO_3)_2HCO_3]^{3-}$ via Hybrid QM/MM MD Simulations
(see page 12938)

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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 $[UO_2(CO_3)_2HCO_3]^{3-}$ 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. Tirler. See page 12938.

Review Article

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13011 Ⓢ 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*

13019 Ⓢ 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

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Ⓢ Supporting Information available via online article