

OCTOBER 16, 2014

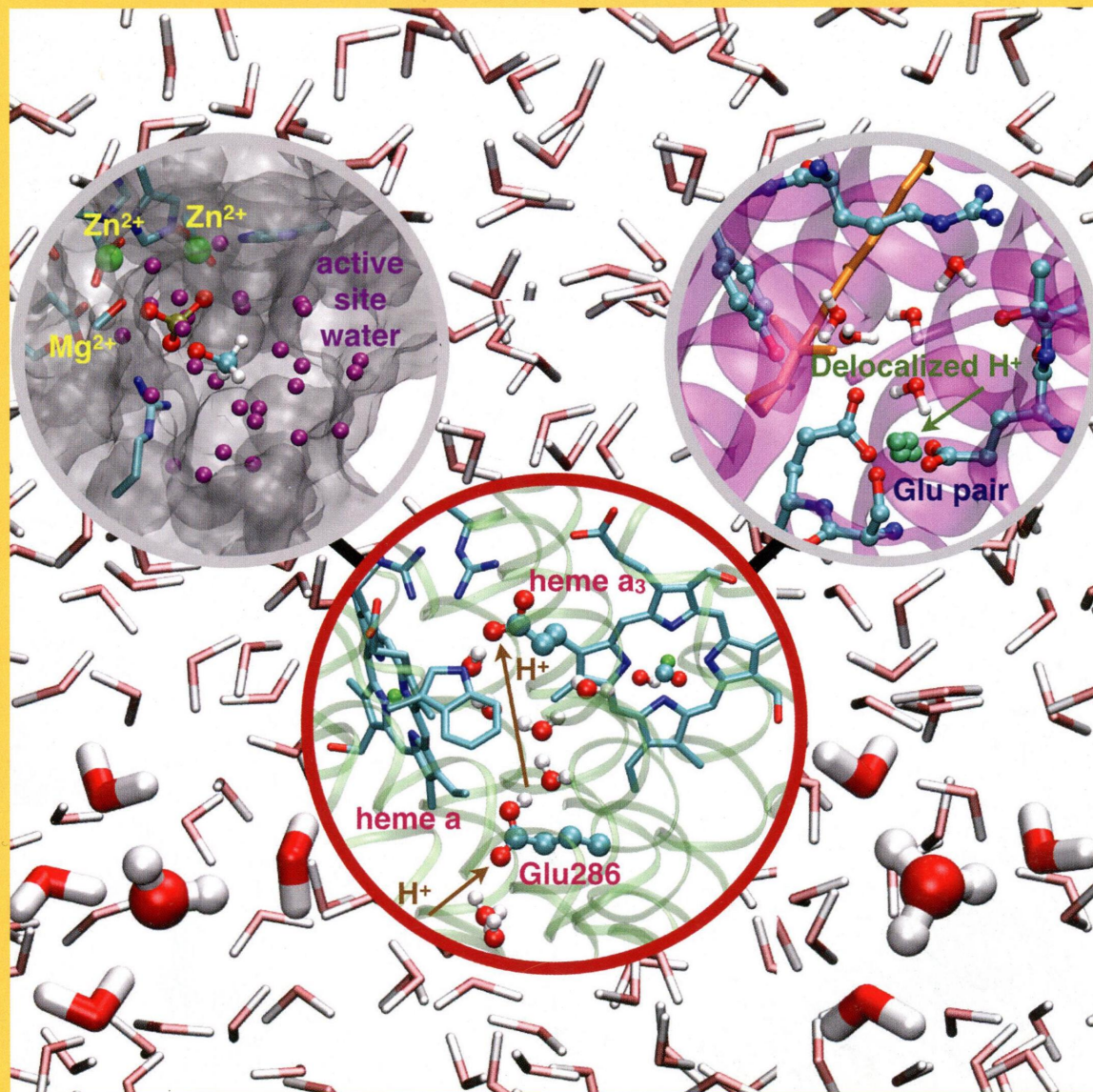
VOLUME 118

NUMBER 41

pubs.acs.org/JPCB

THE JOURNAL OF  
PHYSICAL  
CHEMISTRY

B



Water and the Hydrated Proton in Different Environments: Bulk Water and Protein Interiors (see page 5A)

BIOPHYSICAL CHEMISTRY, BIOMATERIALS, LIQUIDS, AND SOFT MATTER

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**ON THE COVER:** Examples that illustrate recent applications of the DFTB3/MM model where a quantum mechanical description of water proved essential: (clockwise starting from the upper left corner) catalytic specificity and promiscuity in alkaline phosphatase are modulated in part by solvent molecules accessible to the active site; the proton storage site in bacteriorhodopsin involves a proton delocalized between amino acid side chains that are solvated by active site water; proton transfers in cytochrome c oxidase proceed through water wire; and a neutral glutamate near a hydrophobic cavity. See Goyal, P.; Qian, H.-J.; Irle, S.; Lu, X.; Roston, D.; Mori, T.; Elstner, M.; Cui, Q. Molecular Simulation of Water and Hydration Effects in Different Environments: Challenges and Developments for DFTB Based Models. *J. Phys. Chem. B* **2014**, *118* (38), 11007–11027, DOI: 10.1021/jp503372v.

## Articles

### Biophysical Chemistry and Biomolecules

11863 [dx.doi.org/10.1021/jp504518g](https://doi.org/10.1021/jp504518g)

**Not Only Oxidation of Cardiolipin Affects the Affinity of Cytochrome c for Lipid Bilayers**

Cintia Kawai, Juliana C. Ferreira, Mauricio S. Baptista,\* and Iseli L. Nantes\*

11873 [dx.doi.org/10.1021/jp505917p](https://doi.org/10.1021/jp505917p)

**Exciton Circular Dichroism in Channelrhodopsin**

Gennaro Pescitelli,\* Hideaki E. Kato, Satomi Oishi, Jumpei Ito, Andrés Daniel Maturana, Osamu Nureki, and Robert W. Woody\*

11886 [dx.doi.org/10.1021/jp506629y](https://doi.org/10.1021/jp506629y)

**Elucidating the Origin of the Esterase Activity of Human Serum Albumin Using QM/MM Calculations**

Oraphan Phuangsawai, Supa Hannongbua, and M. Paul Gleeson\*

11895 [dx.doi.org/10.1021/jp506733w](https://doi.org/10.1021/jp506733w)

**Sensing Conformational Changes in DNA upon Ligand Binding Using QCM-D. Polyamine Condensation and Rad51 Extension of DNA Layers**

Lu Sun, Karolin Frykholm, Louise H. Fornander, Sofia Svedhem, Fredrik Westerlund, and Björn Åkerman\*

11905 [dx.doi.org/10.1021/jp507154u](https://doi.org/10.1021/jp507154u)

**Local Structural and Environmental Factors Define the Efficiency of an RNA Pseudoknot Involved in Programmed Ribosomal Frameshift Process**

Asmita Gupta and Manju Bansal\*

11921  [dx.doi.org/10.1021/jp508000w](https://doi.org/10.1021/jp508000w)

**Role of Cosolutes in the Aggregation Kinetics of Monoclonal Antibodies**

Lucrèce Nicoud, Margaux Sozo, Paolo Arosio, Andrew Yates, Edith Norrant, and Massimo Morbidelli\*

11931  [dx.doi.org/10.1021/jp508045n](https://doi.org/10.1021/jp508045n)

**NMR and DFT Analysis of Trisaccharide from Heparin Repeating Sequence**

Miloš Hricovini,\* Pierre-Alexandre Driguez, and Olga L. Malkina

11943  [dx.doi.org/10.1021/jp5081498](https://doi.org/10.1021/jp5081498)

**Probing Protein Multidimensional Conformational Fluctuations by Single-Molecule Multiparameter Photon Stamping Spectroscopy**

Maolin Lu and H. Peter Lu\*

11956  [dx.doi.org/10.1021/jp5087152](https://doi.org/10.1021/jp5087152)

**Thermodynamics of Host–Guest Interactions between Fullerenes and a Buckycatcher**

Vu H. Le, Michael Yanney, Matthew McGuire, Andrzej Sygula,\* and Edwin A. Lewis\*

## **Biomaterials, Surfactants, and Membranes**

11965  [dx.doi.org/10.1021/jp5047613](https://doi.org/10.1021/jp5047613)

**Molecular Simulation of the Concentration-Dependent Interaction of Hydrophobic Drugs with Model Cellular Membranes**

Myungshim Kang and Sharon M. Loverde\*

11973  [dx.doi.org/10.1021/jp504853t](https://doi.org/10.1021/jp504853t)

**Reconciling Structural and Thermodynamic Predictions Using All-Atom and Coarse-Grain Force Fields: The Case of Charged Oligo-Arginine Translocation into DMPC Bilayers**

Yuan Hu, Sudipta Kumar Sinha, and Sandeep Patel\*

11993  [dx.doi.org/10.1021/jp5080187](https://doi.org/10.1021/jp5080187)

**Effects of Glucose on Cell Viability and Antioxidant and Anti-inflammatory Properties of Phytochemicals and Phytochemically Modified Membranes**

Teng Chang, Chandrasekaran Neelakandan, Linda DeFine, Thomas Alexander, and Thein Kyu\*

## **Liquids; Chemical and Dynamical Processes in Solution**

12002  [dx.doi.org/10.1021/jp502873z](https://doi.org/10.1021/jp502873z)

**Low-Temperature Solution Growth of ZnO Nanocone/Highly Oriented Nanorod Arrays on Copper**

Yongmei Xia, Youfa Zhang,\* Xinquan Yu,\* and Feng Chen

12008  [dx.doi.org/10.1021/jp5054277](https://doi.org/10.1021/jp5054277)

**Development of a ReaxFF Reactive Force Field for Tetrabutylphosphonium Glycinate/CO<sub>2</sub> Mixtures**

Bo Zhang, Adri C. T. van Duin, and J Karl Johnson\*

12017

[dx.doi.org/10.1021/jp507408r](https://doi.org/10.1021/jp507408r)

**Nanostructure–Thermal Conductivity Relationships in Protic Ionic Liquids**

Thomas Murphy, Luis M. Varela, Grant B. Webber, Gregory G. Warr, and Rob Atkin\*

12025



[dx.doi.org/10.1021/jp507635y](https://doi.org/10.1021/jp507635y)

**Molecular Dynamics Simulations of the Electrospray Process: Formation of NaCl Clusters via the Charged Residue Mechanism**

Lars Konermann,\* Robert G. McAllister, and Haidy Metwally

**Glasses, Colloids, Polymers, and Soft Matter**

12034

[dx.doi.org/10.1021/jp503981p](https://doi.org/10.1021/jp503981p)

**Dissipative Particle Dynamics with an Effective Pair Potential from Integral Equation Theory of Molecular Liquids**

Alexander E. Kobryn, Dragan Nikolić, Olga Lyubimova, Sergey Gusarov, and Andriy Kovalenko\*

12050

[dx.doi.org/10.1021/jp5073796](https://doi.org/10.1021/jp5073796)

**Electrical Mobility of Silver Ion in  $\text{Ag}_2\text{O}-\text{B}_2\text{O}_3-\text{P}_2\text{O}_5-\text{TeO}_2$  Glasses**

Kristina Sklepić, Maryna Vorokhta, Petr Mošner, Ladislav Koudelka, and Andrea Moguš-Milanković\*

12059



[dx.doi.org/10.1021/jp507391j](https://doi.org/10.1021/jp507391j)

**Quantitative Study of Fluctuation Effects by Fast Lattice Monte Carlo Simulations. V. Incompressible Homopolymer Melts**

Pengfei Zhang, Delian Yang, and Qiang Wang\*

12068



[dx.doi.org/10.1021/jp507945t](https://doi.org/10.1021/jp507945t)

**Supramolecular Polymer Transformation: A Kinetic Study**

Jonathan Baram, Haim Weissman, and Boris Rybtchinski\*