

APRIL 16, 2015

VOLUME 119

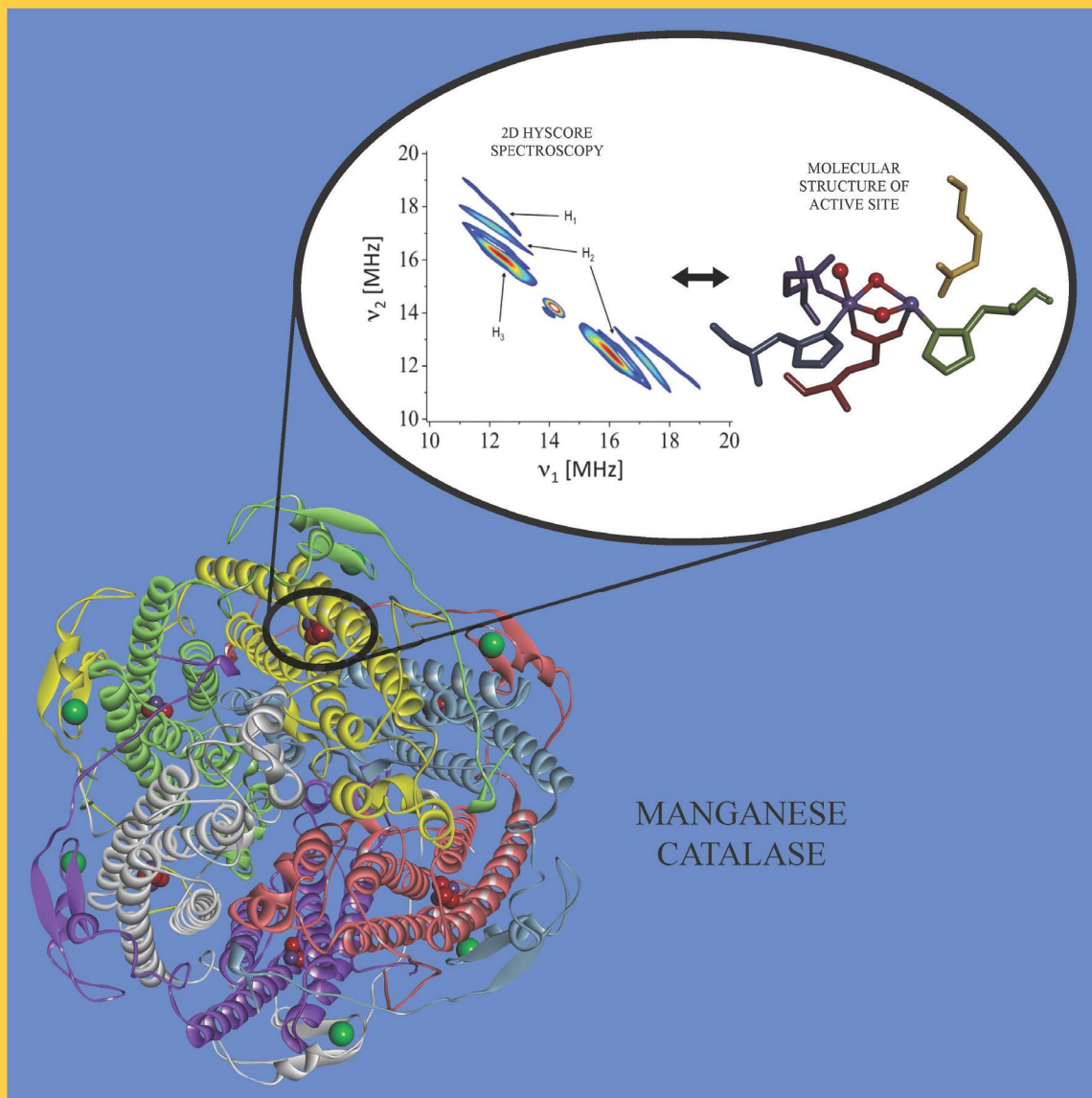
NUMBER 15

pubs.acs.org/JPCB

# THE JOURNAL OF PHYSICAL CHEMISTRY

# B

Structure  
Determination of an  
Enzyme Active Site  
by Two-Dimensional  
Hyperfine Sublevel  
Correlation (HYSCORE)  
Spectroscopy  
(see page 4905)



MANGANESE  
CATALASE

BIOPHYSICAL CHEMISTRY, BIOMATERIALS, LIQUIDS, AND SOFT MATTER



ACS Publications  
Most Trusted. Most Cited. Most Read.

www.acs.org

Content

- 1. Two-Dimensional HYSCORE Spectroscopy of Superoxidized Manganese Catalase: A Model for the Oxygen-Evolving Complex of Photosystem II**  
Christopher S. Coates, Sergey Milikisiyants, Ruchira Chatterjee, Mei M. Whittaker, James W. Whittaker, and K. V. Lakshmi  
*The Journal of Physical Chemistry B* 2015 119 (15), 4905-4916  
DOI: 10.1021/acs.jpcc.5b01602
- 2. Structural Dynamics and Thermostabilization of Neurotensin Receptor 1**  
Sangbae Lee, Supriyo Bhattacharya, Christopher G. Tate, Reinhard Grisshammer, and Nagarajan Vaidehi  
*The Journal of Physical Chemistry B* 2015 119 (15), 4917-4928  
DOI: 10.1021/jp510735f
- 3. Insertion Mechanism and Stability of Boron Nitride Nanotubes in Lipid Bilayers**  
Michael Thomas, Marta Enciso, and Tamsyn A. Hilder  
*The Journal of Physical Chemistry B* 2015 119 (15), 4929-4936  
DOI: 10.1021/acs.jpcc.5b00102
- 4. Twist-Induced Defects of the P-SSP7 Genome Revealed by Modeling the Cryo-EM Density**  
Qian Wang, Christopher G. Myers, and B. Montgomery Pettitt  
*The Journal of Physical Chemistry B* 2015 119 (15), 4937-4943  
DOI: 10.1021/acs.jpcc.5b00865
- 5. Time and Frequency-Domain Measurement of Ground-State Recovery Times in Red Fluorescent Proteins**  
Premashis Manna and Ralph Jimenez  
*The Journal of Physical Chemistry B* 2015 119 (15), 4944-4954  
DOI: 10.1021/acs.jpcc.5b00950
- 6. All-Atomic Simulations on Human Telomeric G-Quadruplex DNA Binding with Thioflavin T**  
Di Luo and Yuguang Mu  
*The Journal of Physical Chemistry B* 2015 119 (15), 4955-4967  
DOI: 10.1021/acs.jpcc.5b01107
- 7. Measurements of Single Nucleotide Electronic States as Nanoelectronic Fingerprints for Identification of DNA Nucleobases, Their Protonated and Unprotonated States, Isomers, and Tautomers**  
Josep Casamada Ribot, Anushree Chatterjee, and Prashant Nagpal  
*The Journal of Physical Chemistry B* 2015 119 (15), 4968-4974  
DOI: 10.1021/acs.jpcc.5b01403
- 8. Twin Displacive Phase Transitions in Amino Acid Quasiracemates**  
Carl Henrik Görbitz and Pavel Karen  
*The Journal of Physical Chemistry B* 2015 119 (15), 4975-4984  
DOI: 10.1021/acs.jpcc.5b01483
- 9. Effect of Cholesterol on the Phase Behavior of Solid-Supported Lipid Vesicle Layers**  
P. Losada-Pérez, M. Khorshid, D. Yongabi, and P. Wagner  
*The Journal of Physical Chemistry B* 2015 119 (15), 4985-4992  
DOI: 10.1021/acs.jpcc.5b00712

- 10. Distinguishing Bicontinuous Lipid Cubic Phases from Isotropic Membrane Morphologies Using <sup>31</sup>P Solid-State NMR Spectroscopy**  
Yu Yang, Hongwei Yao, and Mei Hong  
*The Journal of Physical Chemistry B* **2015** *119* (15), 4993-5001  
DOI: 10.1021/acs.jpcc.5b01001
- 11. DFT Study of the Energetic and Noncovalent Interactions between Imidazolium Ionic Liquids and Hydrofluoric Acid**  
Marco V. Velarde, Marco Gallo, P. A. Alonso, A. D. Miranda, and J. M. Dominguez  
*The Journal of Physical Chemistry B* **2015** *119* (15), 5002-5009  
DOI: 10.1021/acs.jpcc.5b00229
- 12. Vapor–Liquid Equilibrium and Polarization Behavior of the GCP Water Model: Gaussian Charge-on-Spring versus Dipole Self-Consistent Field Approaches to Induced Polarization**  
Ariel A. Chialvo, Filip Moucka, Lukas Vlcek, and Ivo Nezbeda  
*The Journal of Physical Chemistry B* **2015** *119* (15), 5010-5019  
DOI: 10.1021/acs.jpcc.5b00595
- 13. Improving the Hyperpolarization of <sup>31</sup>P Nuclei by Synthetic Design**  
Michael J. Burns, Peter J. Rayner, Gary G. R. Green, Louise A. R. Highton, Ryan E. Mewis, and Simon B. Duckett  
*The Journal of Physical Chemistry B* **2015** *119* (15), 5020-5027  
DOI: 10.1021/acs.jpcc.5b00686
- 14. Thermal and Structural Studies of Imidazolium-Based Ionic Liquids with and without Liquid-Crystalline Phases: The Origin of Nanostructure**  
Fumiya Nemoto, Maiko Kofu, and Osamu Yamamuro  
*The Journal of Physical Chemistry B* **2015** *119* (15), 5028-5034  
DOI: 10.1021/acs.jpcc.5b01080
- 15. Molecular Dynamics Simulations of 2-(Dimethylamino)ethanol (DMEA)**  
Guadalupe Bringas, Pedro Navarro-Santos, Roberto López-Rendón, Jorge López-Lemus, and Fernando Bresme  
*The Journal of Physical Chemistry B* **2015** *119* (15), 5035-5046  
DOI: 10.1021/jp509577x
- 16. Glass Transitions of Poly(methyl methacrylate) Confined in Nanopores: Conversion of Three- and Two-Layer Models**  
Linling Li, Jiao Chen, Weijia Deng, Chen Zhang, Ye Sha, Zhen Cheng, Gi Xue, and Dongshan Zhou  
*The Journal of Physical Chemistry B* **2015** *119* (15), 5047-5054  
DOI: 10.1021/jp511248q
- 17. Effect of Multiwalled Carbon Nanotubes on the Kinetics of the Aniline Polymerization: The Semi-Quantitative OCP Approach**  
Nikolay A. Ogurtsov, Yuriy V. Noskov, and Alexander A. Pud  
*The Journal of Physical Chemistry B* **2015** *119* (15), 5055-5061  
DOI: 10.1021/jp511665q
- 18. In Situ Analysis of Melt-Drawing Behavior of Ultrahigh Molecular Weight Polyethylene Films with Different Molecular Weights: Roles of Entanglements on Oriented Crystallization**  
Satomi Kato, Hidekazu Tanaka, Takeshi Yamanobe, and Hiroki Uehara  
*The Journal of Physical Chemistry B* **2015** *119* (15), 5062-5070  
DOI: 10.1021/jp512246d
- 19. Fast Surface Diffusion of Amorphous o-Terphenyl and Its Competition with Viscous Flow in Surface Evolution**  
Wei Zhang, Caleb W. Brian, and Lian Yu  
*The Journal of Physical Chemistry B* **2015** *119* (15), 5071-5078  
DOI: 10.1021/jp5127464
- 20. Structure and Dynamics of Ionic Micelles: MD Simulation and Neutron Scattering Study**

B. Aoun, V. K. Sharma, E. Pellegrini, S. Mitra, M. Johnson, and R. Mukhopadhyay  
*The Journal of Physical Chemistry B* **2015** *119* (15), 5079-5086  
DOI: 10.1021/acs.jpcc.5b00020

**21. Molecular Motions in Supercooled and Glassy Ibuprofen: Deuteron Magnetic Resonance and High-Resolution Rheology Study**

S. Bauer, M. Storek, C. Gainaru, H. Zimmermann, and R. Böhmer  
*The Journal of Physical Chemistry B* **2015** *119* (15), 5087-5095  
DOI: 10.1021/acs.jpcc.5b01072

**22. Structural Origin of Fragility in Ge–As–S Glasses Investigated by Calorimetry and Raman Spectroscopy**

Yan Yang, Bin Zhang, Anping Yang, Zhiyong Yang, and Pierre Lucas  
*The Journal of Physical Chemistry B* **2015** *119* (15), 5096-5101  
DOI: 10.1021/acs.jpcc.5b01768

**23. Direct Evidence for Secondary Interactions in Planar and Nonplanar Aromatic  $\pi$ -Conjugates and Their Photophysical Characteristics in Solid-State Assemblies**

Mahima Goel, Karnati Narasimha, and Manickam Jayakannan  
*The Journal of Physical Chemistry B* **2015** *119* (15), 5102-5112  
DOI: 10.1021/acs.jpcc.5b01956