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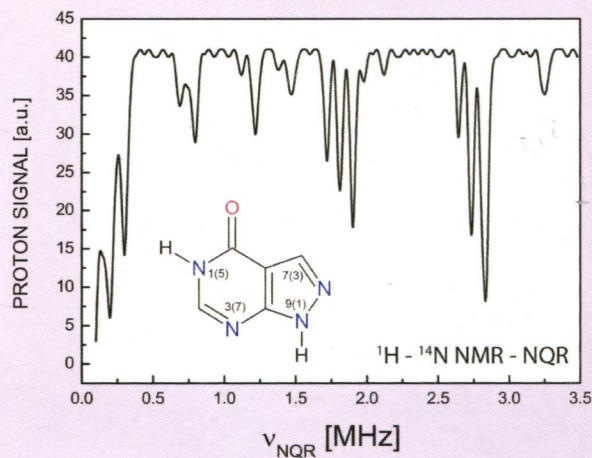
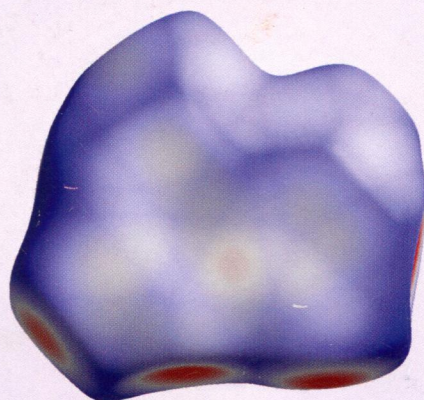
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# THE JOURNAL OF PHYSICAL CHEMISTRY

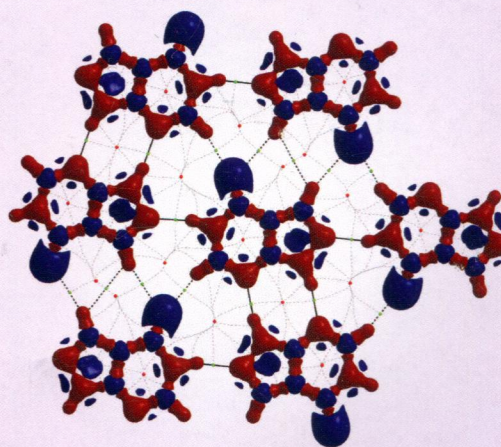
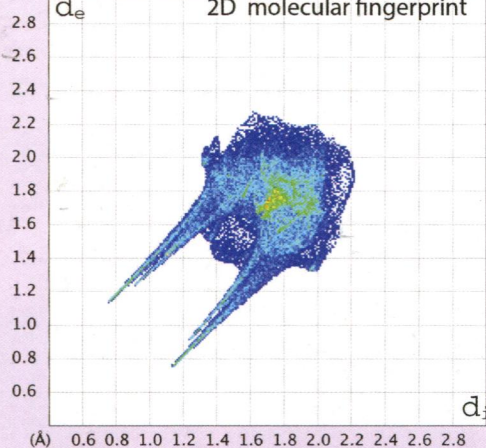
B

3D Hirshfeld surface



Allopurinol, an Old  
New Drug:  $^1\text{H}$ - $^{14}\text{N}$   
NQR, DFT/QTAIM,  
and Hirshfeld  
Surfaces Study  
(see page 10837)

2D molecular fingerprint



DFT/QTAIM Laplacian of electron density

BIOPHYSICAL CHEMISTRY, BIOMATERIALS, LIQUIDS, AND SOFT MATTER



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**ON THE COVER:** An insight into prototropism and supramolecular motifs in the solid-state structure of allopurinol. An example of the use of complementary techniques:  $^1\text{H}$ – $^{14}\text{N}$  NQDR spectrum (top right), hybrid DFT/QTAIM Laplacian of the electron density (bottom right), 3D Hirshfeld Surface (top left), and 2D molecular fingerprint (bottom left). See page 10837.

## Articles

### Biophysical Chemistry and Biomolecules

10813



dx.doi.org/10.1021/jp503915p

#### The Impact of 4-Thiaproline on Polyproline Conformation

Yu-Ju Lin, Chiao-Hsin Chang, and Jia-Cherng Horng\*

10821

dx.doi.org/10.1021/jp504548w

#### Temperature-Dependent Dynamics of Dry and Hydrated $\beta$ -Casein Studied by Quasielastic Neutron Scattering

Gurpreet K Dhindsa, Madhusudan Tyagi, and Xiang-qiang Chu\*

10830



dx.doi.org/10.1021/jp504798s

#### Driving $\beta$ -Strands into Fibrils

Zhaoqian Su and Cristiano L. Dias\*

10837

dx.doi.org/10.1021/jp504871y

#### An Insight into Prototropism and Supramolecular Motifs in Solid-State Structures of Allopurinol, Hypoxanthine, Xanthine, and Uric Acid. A $^1\text{H}$ – $^{14}\text{N}$ NQDR Spectroscopy, Hybrid DFT/QTAIM, and Hirshfeld Surface-Based Study

Jolanta Natalia Latosińska,\* Magdalena Latosińska, Janez Seliger, Veselko Žagar, and Zygmunt Kazimierzczuk

10854



dx.doi.org/10.1021/jp5050546

#### Direct Evidence of Catalytic Heterogeneity in Lactate Dehydrogenase by Temperature Jump Infrared Spectroscopy

Michael J. Reddish, Huo-Lei Peng, Hua Deng, Kunal S. Panwar, Robert Callender, and R. Brian Dyer\*

10863



dx.doi.org/10.1021/jp505180t

#### Functional Water Molecules in Rhodopsin Activation

Xianqiang Sun, Hans Ågren, and Yaoquan Tu\*

**Conformational Preferences of DNA in Reduced Dielectric Environments**

Asli Yildirim, Monika Sharma, Bradley Michael Varner, Liang Fang, and Michael Feig\*

**Analysis of Influenza A Virus NS1 Dimer Interfaces in Solution by Pulse EPR Distance Measurements**

Philip S. Kerry,\* Hannah L. Turkington, Katrin Ackermann, Stephen A. Jameison, and Bela E. Bode\*

**Computational Investigation of Enthalpy–Entropy Compensation in Complexation of Glycoconjugated Bile Salts with  $\beta$ -Cyclodextrin and Analogs**

Kasper D. Tidemand, Christian Schönbeck, René Holm,\* Peter Westh, and Günther H. Peters\*

**Binding of Doxyl Stearic Spin Labels to Human Serum Albumin: An EPR Study**

Aleksandra A. Pavičević, Ana D. Popović-Bijelić, Miloš D. Mojović, Snežana V. Šušnjar, and Goran G. Bačić\*

**Theoretical Study on Excited States of Bacteriochlorophyll  $a$  in Solutions with Density Functional Assessment**

Masahiro Higashi,\* Takahiro Kosugi, Shigehiko Hayashi, and Shinji Saito\*

**Biomaterials, Surfactants, and Membranes****Dynamic Performance of Duolayers at the Air/Water Interface. 1. Experimental Analysis**

Andy H. M. Leung, Emma L. Prime, Diana N. H. Tran, Qiang Fu, Andrew J. Christofferson, George Yiapanis, Irene Yarovsky, Greg G. Qiao,\* and David H. Solomon\*

**Dynamic Performance of Duolayers at the Air/Water Interface. 2. Mechanistic Insights from All-Atom Simulations**

Andrew J. Christofferson, George Yiapanis, Andy H. M. Leung, Emma L. Prime, Diana N. H. Tran, Greg G. Qiao, David H. Solomon, and Irene Yarovsky\*

**Packing Density Changes of Supported Lipid Bilayers Observed by Fluorescence Microscopy and Quartz Crystal Microbalance-Dissipation**

Chiho Kataoka-Hamai\* and Mahoko Higuchi

**Liquids; Chemical and Dynamical Processes in Solution****Effect of Solvent on Diffusion: Probing with Nonpolar Solutes**

T. C. Chan,\* Irene Lee, and K. S. Chan

10956 

[dx.doi.org/10.1021/jp507884w](https://doi.org/10.1021/jp507884w)

**Methane Aqueous Fluids in Montmorillonite Clay Interlayer under Near-Surface Geological Conditions: A Grand Canonical Monte Carlo and Molecular Dynamics Simulation Study**

Qi Rao and Yongsheng Leng\*

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## Glasses, Colloids, Polymers, and Soft Matter

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10966 

[dx.doi.org/10.1021/jp504138r](https://doi.org/10.1021/jp504138r)

**Parallel Optimization of a Reactive Force Field for Polycondensation of Alkoxysilanes**

Joshua D. Deetz\* and Roland Faller\*

10979 

[dx.doi.org/10.1021/jp5041635](https://doi.org/10.1021/jp5041635)

**Thermodynamic Description of Hofmeister Effects on the LCST of Thermosensitive Polymers**

Jan Heyda and Joachim Dzubiella\*

10989 

[dx.doi.org/10.1021/jp504961q](https://doi.org/10.1021/jp504961q)

**Lattice Model for Silica Polymerization: Monte Carlo Simulations of the Transition between Gel and Nanoparticle Phases**


Mohammad Navaid Khan, Scott M. Auerbach,\* and Peter A. Monson\*

11000 

[dx.doi.org/10.1021/jp5056182](https://doi.org/10.1021/jp5056182)

**Size-Dependent Second Virial Coefficients of Quantum Dots from Quantitative Cryogenic Electron Microscopy**

J. van Rijssel, V. F. D. Peters, J. D. Meeldijk, R. J. Kortschot, R. J. A. van Dijk-Moes, A. V. Petukhov, B. H. Ern , and A. P. Philipse\*

 Supporting Information available via online article