

# THE JOURNAL OF PHYSICAL CHEMISTRY

# B

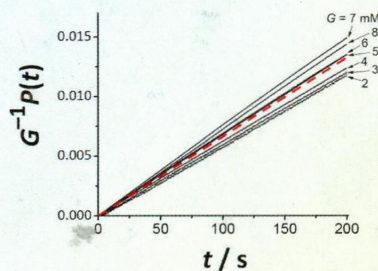
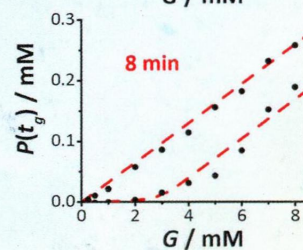
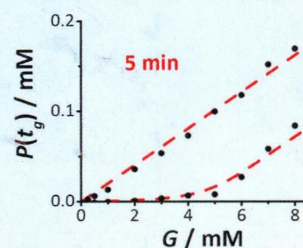
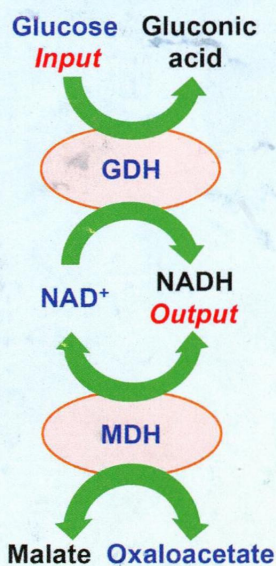
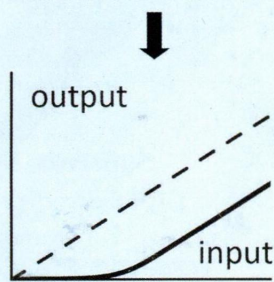
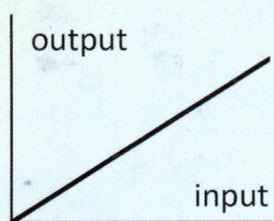
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$$P(t) = RGt - M_0 + \frac{M_0 e^{-K(\frac{1}{2}RGt - M_0)t}}{1 + KM_0 \int_0^t e^{-K(\frac{1}{2}RG\tau - M_0)\tau} d\tau}$$



$$P(t) = RGt - M_0 + \frac{2\sqrt{KRG}M_0 e^{\frac{Kt}{2}(2M_0 - RGt)}}{\sqrt{2\pi}KM_0 e^{\frac{KM_0^2}{2RG}} \left[ \text{erf}\left(\sqrt{\frac{K}{2RG}}M_0\right) - \text{erf}\left(\sqrt{\frac{K}{2RG}}(M_0 - RGt)\right) \right] + 2\sqrt{KRG}}$$

**Model of Threshold Filtering in an Enzymatic Cascade for Bioanalytical and Biocomputing Applications (see page 12435)**

BIOPHYSICAL CHEMISTRY, BIOMATERIALS, LIQUIDS, AND SOFT MATTER



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**ON THE COVER:** Threshold filtering by processes catalyzed by malate dehydrogenase is explained in terms of a model that incorporates an inhibition of this enzyme that has a reversible mechanism of action. Experimental data for a system in which the output signal is produced by biocatalytic processes of the enzyme glucose dehydrogenase are analyzed to verify the model's validity. See page 12435.

## Feature Article


12311 [dx.doi.org/10.1021/jp507763a](http://dx.doi.org/10.1021/jp507763a)  
Design of Controlled Drug Delivery System Based on Disulfide Cleavage Trigger  
Dong Yang, Wulian Chen, and Jianhua Hu\*


## Articles

### Biophysical Chemistry and Biomolecules

12318 [dx.doi.org/10.1021/jp502818u](http://dx.doi.org/10.1021/jp502818u)  
Electron Transfer Dissociation Mass Spectrometry of Peptides Containing Free Cysteine Using Group XII Metals as a Charge Carrier  
Daiki Asakawa\* and Yoshinao Wada

12326  [dx.doi.org/10.1021/jp503972j](http://dx.doi.org/10.1021/jp503972j)  
Molecular Dynamics Simulation of Protein Crystal with Polarized Protein-Specific Force Field  
Yongxiu Li, John Z. H. Zhang, and Ye Mei\*

12336  [dx.doi.org/10.1021/jp504615f](http://dx.doi.org/10.1021/jp504615f)  
Interaction between Metal Cation and Unnatural Peptide Backbone Mediated by Polarized Water Molecules: Study of Infrared Spectroscopy and Computations  
Jipei Shi and Jianping Wang\*

12348  [dx.doi.org/10.1021/jp504997k](http://dx.doi.org/10.1021/jp504997k)  
Dissecting the Dynamic Conformations of the Metamorphic Protein Lymphotactin  
Sophie R. Harvey, Massimiliano Porrini, Albert Konijnenberg, David J. Clarke, Robert C. Tyler, Patrick R. R. Langridge-Smith, Cait E. MacPhee, Brian F. Volkman, and Perdita E. Barran\*

- 12360 dx.doi.org/10.1021/jp5065903  
**Metalization of Single-Stranded PolyI by Zn<sup>2+</sup> Ions in Neutral Solutions**  
Victor A. Sorokin, Vladimir A. Valeev, Evgeniya L. Usenko, and Valery V. Andrushchenko\*
- 12366 dx.doi.org/10.1021/jp506974r  
**Simulation of Two-Dimensional Electronic Spectra of Phycoerythrin 545 at Ambient Temperature**  
Xuan Leng and Xian-Ting Liang\*
- 12371 dx.doi.org/10.1021/jp5072742  
**Vibrational Signatures of S-Nitrosoglutathione as Gaseous, Protonated Species**  
Barbara Gregori, Leonardo Guidoni, Barbara Chiavarino, Debora Scuderi, Edith Nicol, Gilles Frison,\* Simonetta Fornarini, and Maria Elisa Crestoni\*
- 12383 dx.doi.org/10.1021/jp507374q  
**Irreversible Trimer to Monomer Transition of Thermophilic Rhodopsin upon Thermal Stimulation**  
Takashi Tsukamoto, Makoto Demura, and Yuki Sudo\*
- 12395 dx.doi.org/10.1021/jp5075169  
**Molecular Beam and *ab Initio* Studies of Photoactive Yellow Protein Chromophores: Influence of the Thioester Functionality and Single Bond Rotation**  
Eric M. M. Tan, Saeed Amirjalayer, Paul Mazzella, Bert H. Bakker, Jan H. van Maarseveen, Hans Bieraugel, and Wybren J. Buma\*
- 12404 dx.doi.org/10.1021/jp507741r  
**Protein Oligomerization Equilibria and Kinetics Investigated by Fluorescence Correlation Spectroscopy: A Mathematical Treatment**  
David M. Kanno and Marcia Levitus\*
- 12416 dx.doi.org/10.1021/jp507898x  
**Probing the Effect of Ionic Strength on the Functional Robustness of the Triheme Cytochrome PpcA from *Geobacter sulfurreducens*: A Contribution for Optimizing Biofuel Cell's Power Density**  
Joana M. Dantas, Leonor Morgado, Ana C. Marques, and Carlos A. Salgueiro\*
- 12426 dx.doi.org/10.1021/jp5079289  
**Specific Recognition Mechanism between RNA and the KH3 Domain of Nova-2 Protein**  
Qingfen Yu, Wei Ye, Cheng Jiang, Ray Luo,\* and Hai-Feng Chen\*
- 12435 dx.doi.org/10.1021/jp508224y  
**Kinetic Model for a Threshold Filter in an Enzymatic System for Bioanalytical and Biocomputing Applications**  
Vladimir Privman,\* Sergii Domanskyi, Shay Mailloux, Yaovi Holade, and Evgeny Katz\*

12444

[dx.doi.org/10.1021/jp508304h](https://doi.org/10.1021/jp508304h)

**Membrane Potential Bistability in Nonexcitable Cells as Described by Inward and Outward Voltage-Gated Ion Channels**  
Javier Cervera,\* Antonio Alcaraz, and Salvador Mafe\*

## Biomaterials, Surfactants, and Membranes

12451

[dx.doi.org/10.1021/jp507049z](https://doi.org/10.1021/jp507049z)

**Effect of Molecular Orientation on Monolayer and Multilayer Formations of Fluorocarbon Alcohol and Fluorocarbon- $\alpha,\omega$ -diol Mixture at the Hexane/water Interface**

Ryushi Fukuhara, Hajime Tanida, Kiyofumi Nitta, Toshiaki Ina, Tomoya Uruga, Hiroki Matsubara, Makoto Aratono, and Takanori Takiue\*

12462

[dx.doi.org/10.1021/jp507289w](https://doi.org/10.1021/jp507289w)

**Peptides with the Same Composition, Hydrophobicity, and Hydrophobic Moment Bind to Phospholipid Bilayers with Different Affinities**

Melissa A. Cherry, Sarah K. Higgins, Hilary Melroy, Hee-Seung Lee, and Antje Pokorny\*

12471



[dx.doi.org/10.1021/jp507296r](https://doi.org/10.1021/jp507296r)

**Atomistic Description of Fullerene-Based Membranes**

Eudes Eterno Fileti\*

12478



[dx.doi.org/10.1021/jp508312n](https://doi.org/10.1021/jp508312n)

**Low-Temperature Molecular Motions in Lipid Bilayers in the Presence of Sugars: Insights into Cryoprotective Mechanisms**

Konstantin B. Konov, Nikolay P. Isaev, and Sergei A. Dzuba\*

12486

[dx.doi.org/10.1021/jp508430e](https://doi.org/10.1021/jp508430e)

**X-ray Studies of Interfacial Strontium–Extractant Complexes in a Model Solvent Extraction System**

Wei Bu,\* Miroslav Mihaylov, Daniel Amoanu, Binhua Lin, Mati Meron, Ivan Kuzmenko, L. Soderholm,\* and Mark L. Schlossman\*

## Liquids; Chemical and Dynamical Processes in Solution

12501



[dx.doi.org/10.1021/jp506385j](https://doi.org/10.1021/jp506385j)

**Molecular Origin of the Self-Assembled Morphological Difference Caused by Varying the Order of Charged Residues in Short Peptides**

Li Deng, Peng Zhou, Yurong Zhao, Yanting Wang,\* and Hai Xu\*

12511

[dx.doi.org/10.1021/jp506809m](https://doi.org/10.1021/jp506809m)

**pH-Responsive Anionic Wormlike Micelle Based on Sodium Oleate Induced by NaCl**

Hongsheng Lu,\* Qianping Shi, and Zhiyu Huang

12518  [dx.doi.org/10.1021/jp506876v](https://doi.org/10.1021/jp506876v)

**Theoretical Study of Solvent Effects on the Ground and Low-Lying Excited Free Energy Surfaces of a Push–Pull Substituted Azobenzene**

Jose C. Corchado,\* M. Luz Sánchez, Ignacio Fdez. Galván, M. Elena Martín, Aurora Muñoz-Losa, Rute Barata-Morgado, and Manuel A. Aguilar

## Glasses, Colloids, Polymers, and Soft Matter

12531  [dx.doi.org/10.1021/jp507464m](https://doi.org/10.1021/jp507464m)

**Perfluoroalkane Force Field for Lipid Membrane Environments**

Guido Falk von Rudorff, Tobias Watermann, and Daniel Sebastiani\*

12541  [dx.doi.org/10.1021/jp506240j](https://doi.org/10.1021/jp506240j)

**Quenching of the Perylene Fluorophore by Stable Nitroxide Radical-Containing Macromolecules**

Barbara K. Hughes, Wade A. Braunecker, Andrew J. Ferguson, Travis W. Kemper, Ross E. Larsen, and Thomas Gennett\*

12549 [dx.doi.org/10.1021/jp5069818](https://doi.org/10.1021/jp5069818)

**Confined Phase Diagram of Binary *n*-Alkane Mixtures within Three-Dimensional Microcapsules**

Xia Gao, Dongsheng Fu, Baoquan Xie, Yunlan Su,\* and Dujin Wang

12556  [dx.doi.org/10.1021/jp5085789](https://doi.org/10.1021/jp5085789)

**Atomistic Simulations of P(NDI2OD-T2) Morphologies: From Single Chain to Condensed Phases**

Claudia Caddeo,\* Daniele Fazzi, Mario Caironi, and Alessandro Mattoni\*

12566 [dx.doi.org/10.1021/jp508823z](https://doi.org/10.1021/jp508823z)

**High-Precision Temperature Determination of Evaporating Light-Absorbing and Non-Light-Absorbing Droplets**

G. Derkachov,\* D. Jakubczyk, M. Woźniak,\* J. Archer, and M. Kolwas

## Additions and Corrections

12575 [dx.doi.org/10.1021/jp5100796](https://doi.org/10.1021/jp5100796)

**Correction to “Determination of Chain Flip Rates in Poly(ethylene) Crystallites by Solid-State Low-Field <sup>1</sup>H NMR for Two Different Sample Morphologies”**

R. Bärenwald, Y. Champouret, K. Saalwächter,\* and K. Schäler\*