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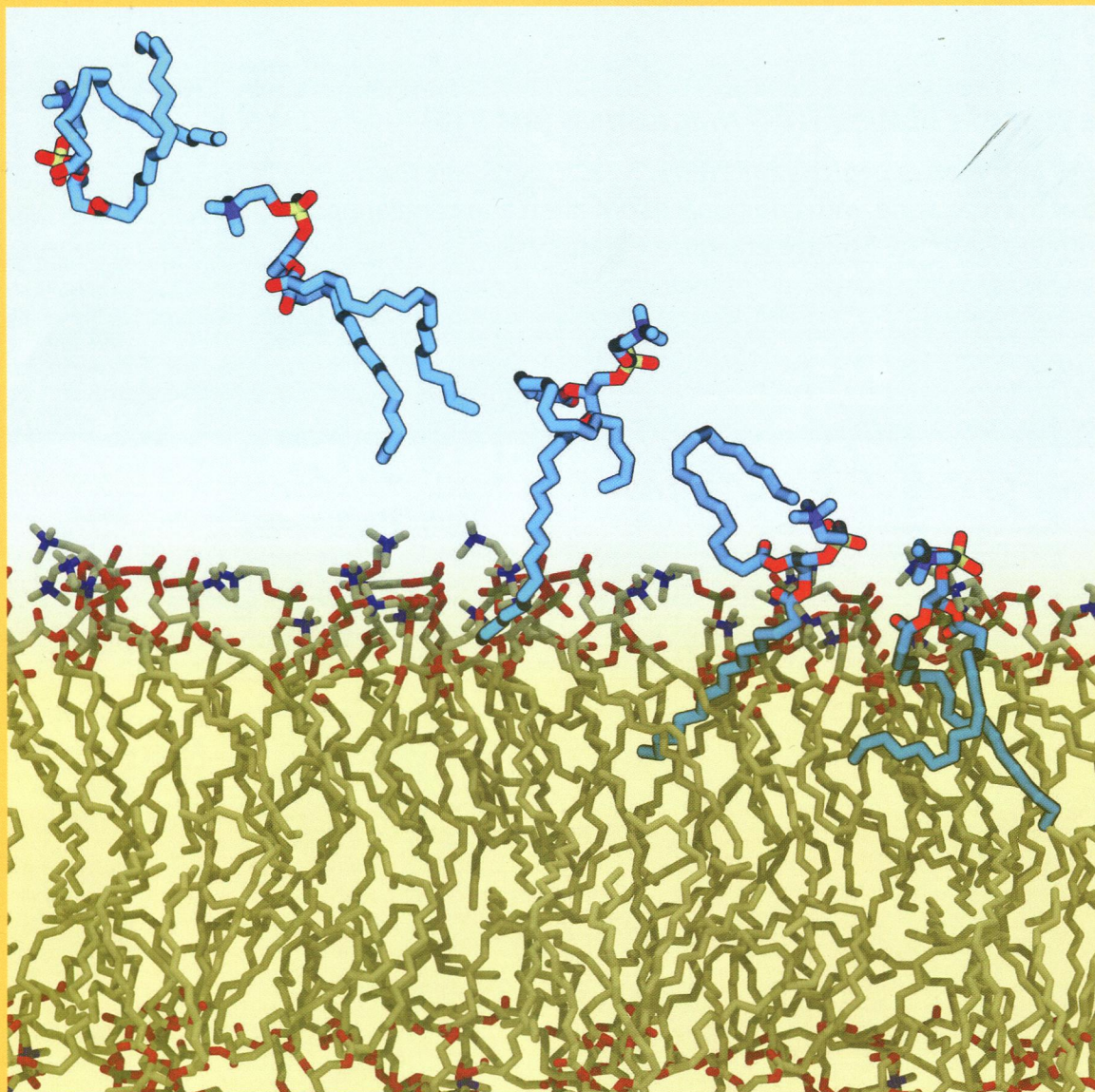
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# THE JOURNAL OF PHYSICAL CHEMISTRY

B

Orchestrated Pathway  
for Phospholipid  
Insertion into  
Biological Membranes  
(see page 5A)



BIOPHYSICAL CHEMISTRY, BIOMATERIALS, LIQUIDS, AND SOFT MATTER



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**ON THE COVER:** Orchestrated pathway for phospholipid insertion into biological membranes. The orchestrated mechanism and pathway for phospholipid insertion into biological membranes progressing from a solvated state (left) to a fully inserted state (right) characterized by molecular dynamics simulations. Spontaneous and reproducible binding and insertion of phospholipids into lipid bilayers captured by equilibrium simulations indicate that, instead of randomly inserting into the membrane, lipid molecules consistently follow a specific insertion pathway/mechanism where each acyl tail independently inserts into the bilayer. The insertion is then completed by the subsequent partitioning of the lipid head group into the membrane. The kinetic model emerging from the analysis of individual insertion steps suggests that the association of the phospholipid to the membrane is the rate-limiting step in this multistaged process. The image was generated in VMD showing only the heavy atoms of the membrane and the inserting phospholipid, with the latter shown in multiple snapshots taken from different time points along the same trajectory. See page 1754.

## Articles

### Biophysical Chemistry and Biomolecules

1707 [dx.doi.org/10.1021/jp407390f](http://dx.doi.org/10.1021/jp407390f)

**Molecular Dynamics Simulations Approach for the Characterization of Peptides with Respect to Hydrophobicity**  
 Sven Amrhein, Stefan Alexander Oelmeier, Florian Dismer, and Jürgen Hubbuch\*

1715 [dx.doi.org/10.1021/jp411178h](http://dx.doi.org/10.1021/jp411178h)

**Self-Aggregation and Optical Absorption of Stilbazolium Merocyanine in Chloroform**  
 Daniel L. Silva,\* N. Arul Murugan, Jacob Kongsted, Hans Ågren, and Sylvio Canuto

1726 [dx.doi.org/10.1021/jp409386t](http://dx.doi.org/10.1021/jp409386t)

**Elucidating Molecular Motion through Structural and Dynamic Filters of Energy-Minimized Conformer Ensembles**  
 Prashant S. Emani, Michael F. Bardaro Jr., Wei Huang, Sergio Aragon, Gabriele Varani, and Gary P. Drobny\*

1743  [dx.doi.org/10.1021/jp4098233](http://dx.doi.org/10.1021/jp4098233)

**Photophysics of Flavin Derivatives Absorbing in the Blue-Green Region: Thioflavins As Potential Cofactors of Photoswitches**  
 Christel M. Marian,\* Setsuko Nakagawa, Vidisha Rai-Constapel, Bora Karasulu, and Walter Thiel


1754  [dx.doi.org/10.1021/jp409854w](http://dx.doi.org/10.1021/jp409854w)

**A Microscopic View of Phospholipid Insertion into Biological Membranes**  
 Josh V. Vermaas and Emad Tajkhorshid\*

1765  [dx.doi.org/10.1021/jp409988n](https://doi.org/10.1021/jp409988n)

**Self-Assembly of an Aspartate-Rich Sequence from the Adenovirus Fiber Shaft: Insights from Molecular Dynamics Simulations and Experiments**

Phanourios Tamamis, Konstantina Terzaki, Michalis Kassinopoulos, Lefteris Mastroggiannis, Estelle Mossou, V. Trevor Forsyth, Edward P. Mitchell, Anna Mitrali,\* and Georgios Archontis\*

1775  [dx.doi.org/10.1021/jp411130n](https://doi.org/10.1021/jp411130n)

**Characterization of Starch Polymorphic Structures Using Vibrational Sum Frequency Generation Spectroscopy**

Lingyan Kong, Christopher Lee, Seong H. Kim,\* and Gregory R. Ziegler\*

1784  [dx.doi.org/10.1021/jp411293r](https://doi.org/10.1021/jp411293r)

**An Isothermal Titration and Differential Scanning Calorimetry Study of the G-Quadruplex DNA–Insulin Interaction**

Christine M. Timmer, Nicole L. Michmerhuizen, Amanda B. Witte, Margaret Van Winkle, Dejian Zhou, and Kumar Sinniah\*

1791  [dx.doi.org/10.1021/jp411812m](https://doi.org/10.1021/jp411812m)

**Reaction Mechanism of Homoprotocatechuate 2,3-Dioxygenase with 4-Nitrocatechol: Implications for the Role of Substrate**

Geng Dong and Wenzhen Lai\*

1799  [dx.doi.org/10.1021/jp4119138](https://doi.org/10.1021/jp4119138)

**Computing Stability Effects of Mutations in Human Superoxide Dismutase 1**

Kasper P. Kepp\*

1813 [dx.doi.org/10.1021/jp412195m](https://doi.org/10.1021/jp412195m)

**Computation of Standard Binding Free Energies of Polar and Charged Ligands to the Glutamate Receptor GluA2**

Germano Heinzelmann, Po-Chia Chen, and Serdar Kuyucak\*

## Biomaterials, Surfactants, and Membranes

1825  [dx.doi.org/10.1021/jp410387e](https://doi.org/10.1021/jp410387e)

**High Field Dynamic Nuclear Polarization NMR with Surfactant Sheltered Biradicals**

Matthew K. Kiesewetter, Vladimir K. Michaelis, Joseph J. Walsh, Robert G. Griffin,\* and Timothy M. Swager\*

## Liquids; Chemical and Dynamical Processes in Solution

1831  [dx.doi.org/10.1021/jp410487a](https://doi.org/10.1021/jp410487a)

**Structure and Dynamics of Benzyl-NX<sub>3</sub> (X = Me, Et) Trifluoromethanesulfonate Ionic Liquids**

Anurag Prakash Sunda, Vishal M. Dhavale, Sreekumar Kurungot, and Arun Venkatnathan\*

1839 [dx.doi.org/10.1021/jp410998f](https://doi.org/10.1021/jp410998f)

**CO<sub>2</sub> Diffusion in Champagne Wines: A Molecular Dynamics Study**

Alexandre Perret, David A. Bonhommeau,\* Gérard Liger-Belair, Thibaud Cours, and Alexander Alijah

1848  [dx.doi.org/10.1021/jp4113552](https://doi.org/10.1021/jp4113552)

**Probing the Interactions between Ionic Liquids and Water: Experimental and Quantum Chemical Approach**

Imran Khan, Kiki A. Kurnia, Fabrice Mutelet, Simão P. Pinho, and João A. P. Coutinho\*

1861  [dx.doi.org/10.1021/jp411385u](https://doi.org/10.1021/jp411385u)

**Ion-Specific Long-Range Correlations on Interfacial Water Driven by Hydrogen Bond Fluctuations**

Shinichi Enami\* and Agustin J. Colussi\*

1867  [dx.doi.org/10.1021/jp411716y](https://doi.org/10.1021/jp411716y)

**Characterization of the Glass Transition of Water Predicted by Molecular Dynamics Simulations Using Nonpolarizable Intermolecular Potentials**

Cara A. Kreck and Ricardo L. Mancera\*

1881  [dx.doi.org/10.1021/jp412339a](https://doi.org/10.1021/jp412339a)

**Urea Induced Unfolding Dynamics of Flavin Adenine Dinucleotide (FAD): Spectroscopic and Molecular Dynamics Simulation Studies from Femto-Second to Nanosecond Regime**

Abhigyan Sengupta, Reman K. Singh, Krishna Gavvala, Raj Kumar Koninti, Arnab Mukherjee,\* and Partha Hazra\*

1891 [dx.doi.org/10.1021/jp4125205](https://doi.org/10.1021/jp4125205)

**Polarity Controlled Reaction Path and Kinetics of Thermal Cis-to-Trans Isomerization of 4-Aminoazobenzene**

Neeraj Kumar Joshi, Masanori Fuyuki, and Akihide Wada\*

1900 [dx.doi.org/10.1021/jp412692d](https://doi.org/10.1021/jp412692d)

**Effect of Bubble Formation on the Dissociation of Methane Hydrate in Water: A Molecular Dynamics Study**

Takuma Yagasaki, Masakazu Matsumoto, Yoshimichi Andoh, Susumu Okazaki, and Hideki Tanaka\*

1907 [dx.doi.org/10.1021/jp500218r](https://doi.org/10.1021/jp500218r)

**Toward Understanding Solute–Solvent Interaction in Room-Temperature Mono- and Dicationic Ionic Liquids: A Combined Fluorescence Spectroscopy and Mass Spectrometry Analysis**

Prabhat Kumar Sahu, Sudhir Kumar Das, and Moly Sarkar\*

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

1916  [dx.doi.org/10.1021/jp409664d](https://doi.org/10.1021/jp409664d)

**Virtual Synthesis of Thermally Cross-Linked Copolymers from a Novel Implementation of Polymeric**

Lauren J. Abbott, Justin E. Hughes, and Coray M. Colina\*

1925 [dx.doi.org/10.1021/jp409797k](https://doi.org/10.1021/jp409797k)

**Phase Behavior and Relative Stability of Malonamide Polymorphs**

Yohann Corvis, Nicolas Guiblin, and Philippe Espeau\*

1932 [dx.doi.org/10.1021/jp410891s](https://doi.org/10.1021/jp410891s)  
**Determination of Structural Characteristics of All-Organic Radical Liquid Crystals Based on Analysis of the Dipole–Dipole Broadened EPR Spectra**

A. Kh. Vorobiev,\* N. A. Chumakova, D. A. Pomogailo, Y. Uchida, K. Suzuki, Y. Noda, and R. Tamura

1943 [dx.doi.org/10.1021/jp4111053](https://doi.org/10.1021/jp4111053)

**IR, Raman, and NMR Studies of the Short-Range Structures of  $0.5\text{Na}_2\text{S} + 0.5[x\text{GeS}_2 + (1-x)\text{PS}_{5/2}]$  Mixed Glass-Former Glasses**

Christian Bischoff, Katherine Schuller, Nathan Dunlap, and Steve W. Martin\*

1954 [dx.doi.org/10.1021/jp411560r](https://doi.org/10.1021/jp411560r)

**Crystal Structure and Vibrational Spectra of Poly(trimethylene terephthalate) from Periodic Density Functional Theory Calculations**

Daria Galimberti and Alberto Milani\*

1962 [dx.doi.org/10.1021/jp411610a](https://doi.org/10.1021/jp411610a)

**Grafting Amphiphilic Brushes onto Halloysite Nanotubes via a Living RAFT Polymerization and Their Pickering Emulsification Behavior**

Yifan Hou, Junqing Jiang, Kai Li, Yanwu Zhang,\* and Jindun Liu