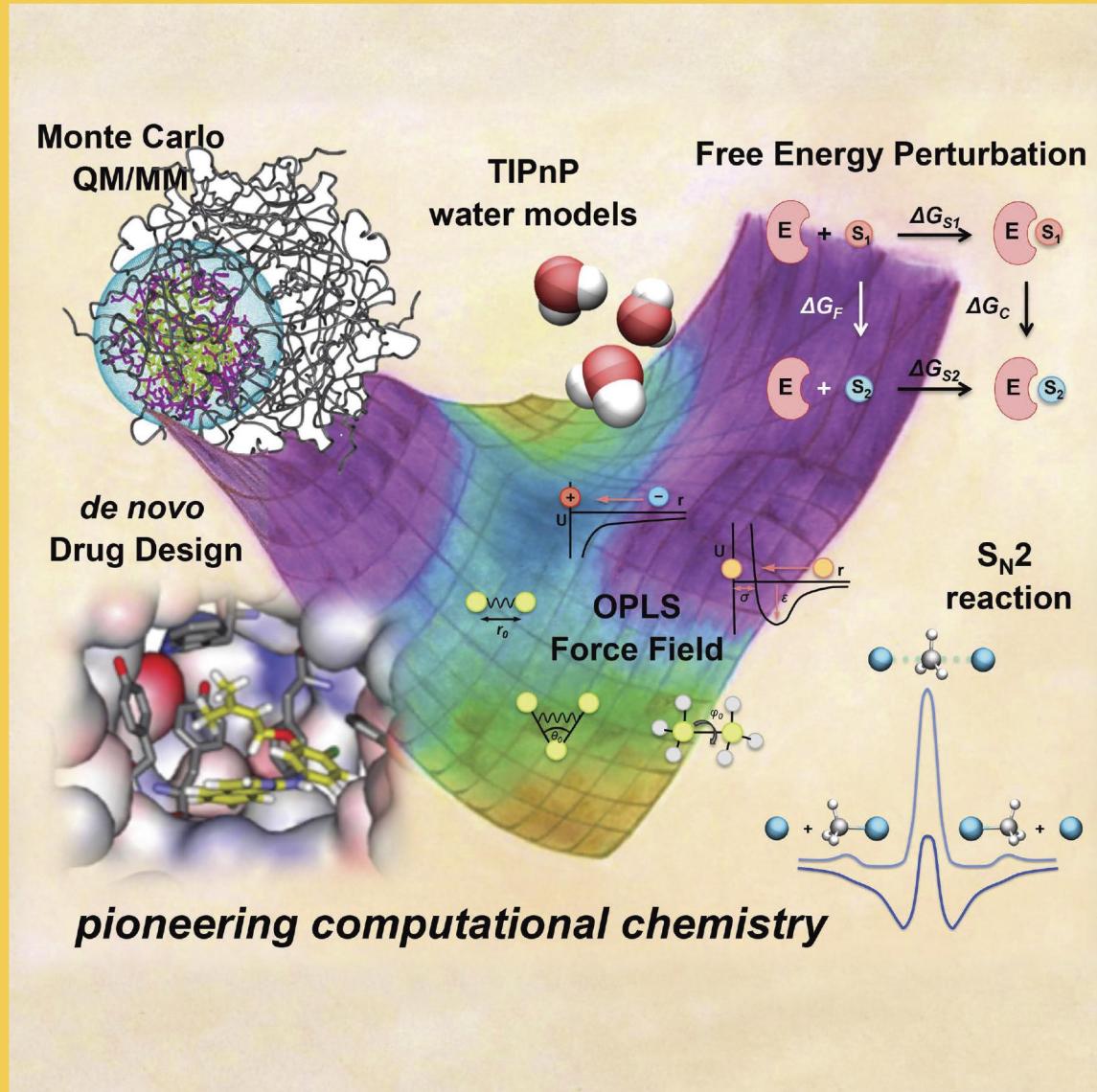


JANUARY 22, 2015  
VOLUME 119  
NUMBER 3  
[pubs.acs.org/JPCB](http://pubs.acs.org/JPCB)

# THE JOURNAL OF PHYSICAL CHEMISTRY B



The cover illustrates the pioneering work in computational chemistry of Prof. Jorgensen, with his main contributions pictorially shown on top of a handmade painting of a potential energy surface (PES).

## WILLIAM L. JORGENSEN FESTSCHRIFT

# THE JOURNAL OF PHYSICAL CHEMISTRY B

January 22, 2015: Vol. 119, Iss. 3

## Content

### 1. Tribute to William L. Jorgensen

Jiali Gao, Modesto Orozco, and Catherine E. Peishoff  
*The Journal of Physical Chemistry B* 2015 119 (3), 621-623

### 2. Autobiography of William L. Jorgensen: Scientific History and Recollections

William L. Jorgensen  
*The Journal of Physical Chemistry B* 2015 119 (3), 624-632

### 3. Group Members of William L. Jorgensen (1975–2014)

*The Journal of Physical Chemistry B* 2015 119 (3), 633-634

### 4. Abbreviated Curriculum Vitae of William L. Jorgensen

*The Journal of Physical Chemistry B* 2015 119 (3), 635-636

### 5. Polarizable Empirical Force Field for Hexopyranose Monosaccharides Based on the Classical Drude Oscillator

Dhilon S. Patel, Xibing He, and Alexander D. MacKerell, Jr.  
*The Journal of Physical Chemistry B* 2015 119 (3), 637-652

### 6. A Tensor-Free Method for the Structural and Dynamical Refinement of Proteins using Residual Dipolar Couplings

Carlo Camilloni and Michele Vendruscolo  
*The Journal of Physical Chemistry B* 2015 119 (3), 653-661

### 7. Computer Simulation Studies of A $\beta$ 37–42 Aggregation Thermodynamics and Kinetics in Water and Salt Solution

Y. Isaac Yang and Yi Qin Gao  
*The Journal of Physical Chemistry B* 2015 119 (3), 662-670

### 8. Atomic Picture of Ligand Migration in Toluene 4-Monoxygenase

Ali Hosseini, Moran Brouk, Maria Fatima Lucas, Fabian Glaser, Ayelet Fishman, and Victor Guallar  
*The Journal of Physical Chemistry B* 2015 119 (3), 671-678

## **9. Solvent-Induced O–H Vibration Red-Shifts of Oxygen-Acids in Hydrogen-Bonded O–H···Base Complexes**

Sharon Keinan, Dina Pines, Philip M. Kiefer, James T. Hynes, and Ehud Pines  
*The Journal of Physical Chemistry B* 2015 119 (3), 679-692

## **10. Hydrogen-Tunneling in Biologically Relevant Small Molecules: The Rotamerizations of $\alpha$ -Ketocarboxylic Acids**

Dennis Gerbig and Peter R. Schreiner  
*The Journal of Physical Chemistry B* 2015 119 (3), 693-703

## **11. Direct QM/MM Excited-State Dynamics of Retinal Protonated Schiff Base in Isolation and Methanol Solution**

Chutintorn Punwong, Jane Owens, and Todd J. Martínez  
*The Journal of Physical Chemistry B* 2015 119 (3), 704-714

## **12. Steered Quantum Dynamics for Energy Minimization**

Micheline Soley, Andreas Markmann, and Victor S. Batista  
*The Journal of Physical Chemistry B* 2015 119 (3), 715-727

## **13. Intricate Internal Rotation Surface and Fundamental Infrared Transitions of the n-Propyl Radical**

Chenyang Li, Jay Agarwal, Chia-Hua Wu, Wesley D. Allen, and Henry F. Schaefer, III  
*The Journal of Physical Chemistry B* 2015 119 (3), 728-735

## **14. A Time-Independent Free Energy Estimator for Metadynamics**

Pratyush Tiwary and Michele Parrinello  
*The Journal of Physical Chemistry B* 2015 119 (3), 736-742

## **15. Ionic Liquid Effects on Nucleophilic Aromatic Substitution Reactions from QM/MM Simulations**

Caley Allen, Billy W. McCann, and Orlando Acevedo  
*The Journal of Physical Chemistry B* 2015 119 (3), 743-752

## **16. Challenge of Representing Entropy at Different Levels of Resolution in Molecular Simulation**

Wei Huang and Wilfred F. van Gunsteren  
*The Journal of Physical Chemistry B* 2015 119 (3), 753-763

## **17. Interactions of Lipids and Detergents with a Viral Ion Channel Protein: Molecular Dynamics Simulation Studies**

Sarah L. Rouse and Mark S. P. Sansom  
*The Journal of Physical Chemistry B* 2015 119 (3), 764-772

## **18. Binding Site Preorganization and Ligand Discrimination in the Purine Riboswitch**

Johan Sund, Christoffer Lind, and Johan Åqvist  
*The Journal of Physical Chemistry B* 2015 119 (3), 773-782

## **19. Hydrogen-Atom Abstraction from a Model Amino Acid: Dependence on the Attacking Radical**

Ruth I. J. Amos, Bun Chan, Christopher J. Easton, and Leo Radom  
*The Journal of Physical Chemistry B* 2015 119 (3), 783-788

## **20. Anandamide Hydrolysis in FAAH Reveals a Dual Strategy for Efficient Enzyme-Assisted Amide Bond Cleavage via Nitrogen Inversion**

Giulia Palermo, Pablo Campomanes, Andrea Cavalli, Ursula Rothlisberger, and Marco De Vivo  
*The Journal of Physical Chemistry B* 2015 119 (3), 789-801

## **21. Solvent Effects on Isotope Effects: Methyl Cation as a Model System**

Philippe B. Wilson, Paul J. Weaver, Ian R. Greig, and Ian H. Williams  
*The Journal of Physical Chemistry B* 2015 119 (3), 802-809

## **22. Automatic GROMACS Topology Generation and Comparisons of Force Fields for Solvation Free Energy Calculations**

Magnus Lundborg and Erik Lindahl  
*The Journal of Physical Chemistry B* 2015 119 (3), 810-823

## **23. Docking and Free Energy Perturbation Studies of Ligand Binding in the Kappa Opioid Receptor**

Dahlia A. Goldfeld, Robert Murphy, Byungchan Kim, Lingle Wang, Thijs Beuming, Robert Abel, and Richard A. Friesner  
*The Journal of Physical Chemistry B* 2015 119 (3), 824-835

## **24. Optimizing Potentials for a Liquid Mixture: A New Force Field for a tert-Butanol and Water Solution**

Michele Di Pierro, Mauro L. Mugnai, and Ron Elber  
*The Journal of Physical Chemistry B* 2015 119 (3), 836-849

## **25. Theoretical Insight into the Relationship between the Structures of Antimicrobial Peptides and Their Actions on Bacterial Membranes**

Licui Chen, Xiaoxu Li, Lianghui Gao, and Weihai Fang  
*The Journal of Physical Chemistry B* 2015 119 (3), 850-860

## **26. Protocols Utilizing Constant pH Molecular Dynamics to Compute pH-Dependent Binding Free Energies**

M. Olivia Kim, Patrick G. Blachly, Joseph W. Kaus, and J. Andrew McCammon  
*The Journal of Physical Chemistry B* 2015 119 (3), 861-872

## **27. Linking Electrostatic Effects and Protein Motions in Enzymatic Catalysis. A Theoretical Analysis of Catechol O-Methyltransferase**

Rafael García-Meseguer, Kirill Zinovjev, Maite Roca, Javier J. Ruiz-Pernía, and Iñaki Tuñón  
*The Journal of Physical Chemistry B* 2015 119 (3), 873-882

## **28. Parameterization of Highly Charged Metal Ions Using the 12-6-4 LJ-Type Nonbonded Model in Explicit Water**

Pengfei Li, Lin Frank Song, and Kenneth M. Merz, Jr.  
*The Journal of Physical Chemistry B* 2015 119 (3), 883-895

## **29. Disordered Structural Ensembles of Vasopressin and Oxytocin and Their Mutants**

Eugene Yedvabny, Paul S. Nerenberg, Clare So, and Teresa Head-Gordon  
*The Journal of Physical Chemistry B* 2015 119 (3), 896-905

## **30. Free Energy Simulations of Active-Site Mutants of Dihydrofolate Reductase**

Dvir Doron, Vanja Stojković, Lokesh Gakhar, Alexandra Vardi-Kilshtain, Amnon Kohen, and Dan Thomas Major  
*The Journal of Physical Chemistry B* 2015 119 (3), 906-916

## **31. Binding Isotope Effects as a Tool for Distinguishing Hydrophobic and Hydrophilic Binding Sites of HIV-1 RT**

Agnieszka Krzemińska, Piotr Paneth, Vicent Moliner, and Katarzyna Świderek  
*The Journal of Physical Chemistry B* 2015 119 (3), 917-927

## **32. Photoinduced Intramolecular Charge Transfer in an Electronically Modified Flavin Derivative: Roseoflavin**

Bora Karasulu and Walter Thiel  
*The Journal of Physical Chemistry B* 2015 119 (3), 928-943

## **33. Role of Hydrophilicity and Length of Diblock Arms for Determining Star Polymer Physical Properties**

Lisa E. Felberg, David H. Brookes, Teresa Head-Gordon, Julia E. Rice, and William C. Swope  
*The Journal of Physical Chemistry B* 2015 119 (3), 944-957

**34. Electronic Absorption Spectra and Solvatochromic Shifts by the Vertical Excitation Model: Solvated Clusters and Molecular Dynamics Sampling**

Aleksandr V. Marenich, Christopher J. Cramer, and Donald G. Truhlar  
*The Journal of Physical Chemistry B* 2015 119 (3), 958-967

**35. Rapid Alchemical Free Energy Calculation Employing a Generalized Born Implicit Solvent Model**

Katja Ostermeir and Martin Zacharias  
*The Journal of Physical Chemistry B* 2015 119 (3), 968-975

**36. Distinguishing Binders from False Positives by Free Energy Calculations: Fragment Screening Against the Flap Site of HIV Protease**

Nanjie Deng, Stefano Forli, Peng He, Alex Perryman, Lauren Wickstrom, R. S. K. Vijayan, Theresa Tiefenbrunn, David Stout, Emilio Gallicchio, Arthur J. Olson, and Ronald M. Levy  
*The Journal of Physical Chemistry B* 2015 119 (3), 976-988

**37. Evolution Alters the Enzymatic Reaction Coordinate of Dihydrofolate Reductase**

Jean E. Masterson and Steven D. Schwartz  
*The Journal of Physical Chemistry B* 2015 119 (3), 989-996

**38. Combined Quantum Mechanics/Molecular Mechanics (QM/MM) Simulations for Protein–Ligand Complexes: Free Energies of Binding of Water Molecules in Influenza Neuraminidase**

Christopher J. Woods, Katherine E. Shaw, and Adrian J. Mulholland  
*The Journal of Physical Chemistry B* 2015 119 (3), 997-1001

**39. Exploring a Non-ATP Pocket for Potential Allosteric Modulation of PI3K $\alpha$**

Paraskevi Gkeka, Alexandra Papafotika, Savvas Christofidis, and Zoe Cournia  
*The Journal of Physical Chemistry B* 2015 119 (3), 1002-1016

**40. Direct Validation of the Single Step Classical to Quantum Free Energy Perturbation**

Christopher Cave-Ayland, Chris-Kriton Skylaris, and Jonathan W. Essex  
*The Journal of Physical Chemistry B* 2015 119 (3), 1017-1025

**41. Multi-Conformer Ensemble Docking to Difficult Protein Targets**

Sally R. Ellingson, Yinglong Miao, Jerome Baudry, and Jeremy C. Smith  
*The Journal of Physical Chemistry B* 2015 119 (3), 1026-1034

## **42. Residue-Specific Force Field Based on Protein Coil Library. RSFF2: Modification of AMBER ff99SB**

Chen-Yang Zhou, Fan Jiang, and Yun-Dong Wu  
*The Journal of Physical Chemistry B* 2015 119 (3), 1035-1047

## **43. Biophysical Characteristics of Cholera Toxin and Escherichia coli Heat-Labile Enterotoxin Structure and Chemistry Lead to Differential Toxicity**

John W. Craft, Jr., Tsai-wei Shen, Lindsey M. Brier, and James M. Briggs  
*The Journal of Physical Chemistry B* 2015 119 (3), 1048-1061

## **44. Parametrization of DFTB3/3OB for Magnesium and Zinc for Chemical and Biological Applications**

Xiya Lu, Michael Gaus, Marcus Elstner, and Qiang Cui  
*The Journal of Physical Chemistry B* 2015 119 (3), 1062-1082

## **45. Pharmacophore-Based Similarity Scoring for DOCK**

Lingling Jiang and Robert C. Rizzo  
*The Journal of Physical Chemistry B* 2015 119 (3), 1083-1102

## **46. Enzymatic Minimum Free Energy Path Calculations Using Swarms of Trajectories**

Melchor Sanchez-Martinez, Martin Field, and Ramon Crehuet  
*The Journal of Physical Chemistry B* 2015 119 (3), 1103-1113

## **47. Motions and Entropies in Proteins as Seen in NMR Relaxation Experiments and Molecular Dynamics Simulations**

Olof Allnér, Nicolas Foloppe, and Lennart Nilsson  
*The Journal of Physical Chemistry B* 2015 119 (3), 1114-1128

## **48. The Adaptive Biasing Force Method: Everything You Always Wanted To Know but Were Afraid To Ask**

Jeffrey Comer, James C. Gumbart, Jérôme Hénin, Tony Lelièvre, Andrew Pohorille, and Christophe Chipot  
*The Journal of Physical Chemistry B* 2015 119 (3), 1129-1151

## **49. Aqueous Transition-Metal Cations as Impurities in a Wide Gap Oxide: The Cu<sup>2+</sup>/Cu<sup>+</sup> and Ag<sup>2+</sup>/Ag<sup>+</sup> Redox Couples Revisited**

Xiandong Liu, Jun Cheng, and Michiel Sprik  
*The Journal of Physical Chemistry B* 2015 119 (3), 1152-1163

## **50. Assessing the Suitability of the Multilevel Strategy for the Conformational Analysis of Small Ligands**

Jordi Juárez-Jiménez, Xavier Barril, Modesto Orozco, Ramon Pouplana, and F. Javier Luque  
*The Journal of Physical Chemistry B* 2015 119 (3), 1164-1172

**51. Hydrogen-Bonded Water Molecules in the M2 Channel of the Influenza A Virus Guide the Binding Preferences of Ammonium-Based Inhibitors**

Eleonora Gianti, Vincenzo Carnevale, William F. DeGrado, Michael L. Klein, and Giacomo Fiorin  
*The Journal of Physical Chemistry B* 2015 119 (3), 1173-1183

**52. Intramolecular Charge-Assisted Hydrogen Bond Strength in Pseudochair Carboxyphosphate**

Sarah E. Kochanek, Traci M. Clymer, Venkata S. Pakkala, Sebastien P. Hebert, Kyle Reeping, Steven M. Firestone, and Jeffrey D. Evanseck  
*The Journal of Physical Chemistry B* 2015 119 (3), 1184-1191

**53. Profiling Transition-State Configurations on the *Trypanosoma cruzi* trans-Sialidase Free-Energy Reaction Surfaces**

Ian L. Rogers and Kevin J. Naidoo  
*The Journal of Physical Chemistry B* 2015 119 (3), 1192-1201

**54. Can Gap Tuning Schemes of Long-Range Corrected Hybrid Functionals Improve the Description of Hyperpolarizabilities?**

Alejandro J. Garza, Osman I. Osman, Abdullah M. Asiri, and Gustavo E. Scuseria  
*The Journal of Physical Chemistry B* 2015 119 (3), 1202-1212

**55. Projected Hybrid Orbitals: A General QM/MM Method**

Yingjie Wang and Jiali Gao  
*The Journal of Physical Chemistry B* 2015 119 (3), 1213-1224

**56. Why Bound Amantadine Fails to Inhibit Proton Conductance According to Simulations of the Drug-Resistant Influenza A M2 (S31N)**

Mitchell L. Gleed and David D. Busath  
*The Journal of Physical Chemistry B* 2015 119 (3), 1225-1231