

Huan-Xiang Zhou

Departments of Chemistry and Physics, University of Illinois at Chicago, Chicago, IL 60607

Education

Ph. D., 1988, Department of Physics, Drexel University

B. S., 1984, Department of Physics, Wuhan University, China

Employment

2017-, Professor and LAS Endowed Chair in the Natural Sciences, Departments of Chemistry and Physics, University of Illinois at Chicago

2005-2017, Professor, Department of Physics, Florida State University

2002-2005, Associate Professor, Department of Physics, Florida State University

1998-2002, Associate Professor, Department of Physics, Drexel University

1995-1998, Assistant Professor, Department of Biochemistry, Hong Kong Univ Sci & Tech

1990-1995, Visiting Associate, Laboratory of Chemical Physics, NIH

1988-1990, Visiting Fellow, Laboratory of Chemical Physics, NIH

Honors

2015, PAI Award for Excellence in Teaching and Research, Florida State University

2011, Distinguished Research Professor

2010, Elected Fellow of the American Physical Society

2008, Elected Fellow of the American Association for the Advancement of Science

1997, Emerson Fellowship, Emory University

1984-1988, CUSPEA Graduate Fellowship, Drexel University

Professional Activities (selected)

2003-, Standing and ad hoc member of MSFD, F04-D, MABS, and BBKA Study Sections

2016-, Biophysics Subject Editor, Elsevier's Life Science Reference Module

2014-, Editorial Board, Protein Engineering, Design and Selection

2008-, Editor-in-Chief, PMC Biophysics; Section Editor, BMC Biophysics

1998-2015, Associate Editor, Cell Biochemistry and Biophysics

2018, Organizing Committee, 4th Biological Diffusion and Brownian Dynamics Brainstorm

2012, Co-Chair, Biophysical Society Biopolymers in Vivo Subgroup Symposium

2010, Co-Chair, Biophysical Society IDP Subgroup Symposium

2009 & 2011, Organizer, Telluride Workshop on Macromolecular Crowding

2009, Organizer, ACS Symposium on Protein Dynamics and Function

Research Interests

Quantitative understanding of biological processes in the cellular context, based on physical principles.

(1) Physical basis of protein liquid-liquid phase separation; (2) Binding kinetics of intrinsically disordered proteins; (3) Structures and functional mechanisms of ion channels and other membrane proteins; and (4) Structures and mechanisms of peptide self-assembly.

Current Grants

Principal Investigator, NIH Grant R35 GM118091, *Quantitative, Mechanistic Studies of Biomolecular Recognition* (2016-2021).

Principal Investigator, NIH Grant R35 3R35GM118091-03S1, *Administrative Supplement to Acquire an Advanced Optical Tweezers Instrument* (2018-2021).

Principal Investigators with Gideon Schreiber, United States-Israel Binational Science Foundation Grant 2015376, *Computational and Experimental Studies on the Complexity of Protein Complex Formation in the Cell in Relation to the Test Tube* (2016-2020).

Co-Principal Investigator, NIH Grant R01 NS088479, *Gating and Permeation in Ionotropic Glutamate Receptors* (2019-2024) (PI: Lonnie Wollmuth).

Co-Principal Investigator, NIH Grant R01 AG045703, *Solid State NMR Structural Analysis of Oligomeric Alzheimer's Beta-Amyloid Peptide* (2014-2020) (PI: Anant Paravastu).

Co-Principal Investigator, NIH Grant R01 AI119178, *Membrane Protein Structures and Interactions in the M. tuberculosis Divisome* (2015-2020) (PI: Tim Cross).

Patent

M. Sharma, M. Yi, H. Dong, H. Qin, D. D. Busath, H.-X. Zhou, and T. A. Cross, *Membrane Proteins, Mechanisms of Action and Uses Thereof*, US Patent 8,581,584 issued on 11/12/2013.

Publications

254. Qin and H.-X. Zhou (2019). *Calculation of second virial coefficients of atomistic proteins using fast Fourier transform*. J. Phys. Chem. B **123**, 8203-8215.
253. A. Ghosh, K. Mazarakos, and H.-X. Zhou (2019). *Three archetypical classes of macromolecular regulators of protein liquid-liquid phase separation*. Proc. Natl. Acad. Sci. USA **116**, 19474-19483.
252. V. Nguemaha, S. Qin, and H.-X. Zhou (2019). *Transfer free energies of test proteins into crowded protein solutions have simple dependence on crowder concentration*. Front. Mol. Biosci. **6**, 39.
251. A. Ghosh, P. E. S. Smith, S. Qin, M. Yi, and H.-X. Zhou (2019). *Both ligands and macromolecular crowders preferentially bind to closed conformations of maltose binding protein*. Biochemistry **58**, 2208-2217.
250. D. Wu and H.-X. Zhou (2019). *Designed mutations alter the binding pathways of an intrinsically disordered protein*. Sci. Rep. **9**, 6172.
249. J. Paulino, X. Pang, I. Hung, H.-X. Zhou, T. A. Cross (2019). *Influenza A M2 channel clustering at high protein to lipid ratios: viral budding implications*. Biophys. J. **116**, 1075-1084.
248. C. Guo and H.-X. Zhou (2019). *Fatty acids compete with β in binding to serum albumin by quenching its conformational flexibility*. Biophys. J. **116**, 248-257.
247. V. Nguemaha, S. Qin, and H.-X. Zhou (2018). *Atomistic modeling of intrinsically disordered proteins under PEG crowding: quantitative comparison with experimental data and implication of protein-crowder attraction*. J. Phys. Chem. B **122**, 11262-11270.
246. J. B. Amin, X. Leng, A. Gochman, H.-X. Zhou, and L. P. Wollmuth (2018). *A conserved glycine harboring disease-associated mutations permits NMDA receptor slow deactivation and high Ca^{2+} permeability*. Nat. Commun. **9**, 3748.
245. A. Hicks and H.-X. Zhou (2018). *Temperature-induced collapse of a disordered peptide observed by three sampling methods in molecular dynamics simulations*. J. Chem. Phys. **149**, 072313.
244. H.-X. Zhou, V. Nguemaha, K. Mazarakos, and S. Qin (2018). *Why do disordered and structured proteins behave differently in phase separation?* Trends Biochem. Sci. **43**, 499-516.
243. V. Nguemaha and H.-X. Zhou (2018). *Liquid-liquid phase separation of patchy particles illuminates diverse effects of regulatory components on protein droplet formation*. Sci. Rep. **8**, 6728.
242. P. Campitelli, J. Guo, H.-X. Zhou, and S. B. Ozkan (2018). *A hinge-shift mechanism modulates allosteric regulations in human Pin1*. J. Phys. Chem. B. **122**, 5623-5629.
241. A. Banks, S. Qin, K. L. Weiss, C. B. Stanley, and H.-X. Zhou (2018). *Intrinsically disordered protein exhibits both compaction and expansion under macromolecular crowding*. Biophys. J. **114**, 1067-1079.
240. H.-X. Zhou and X. Pang (2018). *Electrostatic interactions in protein structure, folding, binding, and condensation*. Chem. Rev. **118**, 1691-1741.
239. T. H. Nguyen, H.-X. Zhou, and D. D. L. Minh (2018). *Using the fast Fourier transform in binding free energy calculations*. J. Comput. Chem. **39**, 621-636.

- 238.L. Ou, M. Matthews, X. Pang, and H.-X. Zhou (2017). *The dock-and-coalesce mechanism for the association of a WASP disordered region with the Cdc42 GTPase*. FEBS. J. **284**, 3381-3391.
- 237.X. Pang and H.-X. Zhou (2017). *Structural modeling for the open state of an NMDA receptor*. J. Struct. Biol. **200**, 369-375.
- 236.J. Amin, C. L. Salussolia, K. Chan, M. C. Regan, J. Dai, H.-X. Zhou, H. Furukawa, M. E. Bowen, and L. P. Wollmuth (2017). *Divergent roles of a peripheral transmembrane segment in AMPA and NMDA receptors*. J. Gen. Physiol. **149**, 661-680.
- 235.H.-X. Zhou (2017). *Gating motions and stationary gating properties of ionotropic glutamate receptors: computation meets electrophysiology*. Acc. Chem. Res. **50**, 814-822.
- 234.H.-X. Zhou and L. P. Wollmuth (2017). *Advancing NMDA receptor physiology by integrating multiple approaches*. Trends Neurosci. **40**, 129-137.
- 233.X. Pang and H.-X. Zhou (2017). *Rate constants and mechanisms of protein-ligand binding*. Annu. Rev. Biophys. **46**, 105-130.
- 232.S. Qin and H.-X. Zhou (2017). *Protein folding, binding, and droplet formation in cell-like conditions*. Curr. Opin. Struct. Biol. **43**, 28-37.
- 231.H.-X. Zhou (2017). *Biophysics: past, present, and future*. In Reference Module in Life Sciences: Elsevier.
- 230.C. Guo and H.-X. Zhou (2016). *Unidirectional allostery in the regulatory subunit R1a facilitates efficient deactivation of protein kinase A*. Proc. Natl. Acad. Sci. USA **113**, E6776-E6785.
- 229.J. Guo and H.-X. Zhou (2016). *Allosteric activation of SENP1 by SUMO1 β -grasp domain involves a dock-and-coalesce mechanism*. eLife **5**, e18249.
- 228.J. Dai and H.-X. Zhou (2016). *Semiclosed conformations of the ligand-binding domains of NMDA receptors during stationary gating*. Biophys. J. **111**, 1418-1428.
- 227.S. Qin and H.-X. Zhou (2016). *Fast method for computing chemical potentials and liquid-liquid phase equilibria of macromolecular solutions*. J. Phys. Chem. B. **120**, 8164-8174.
- 226.W. Im, J. Liang, A. Olson, H.-X. Zhou, S. Vajda, and I. A. Vakser (2016). *Challenges in structural approaches to cell modeling*. J. Mol. Biol. **428**, 2943-2964.
- 225.J. Batra, H. Tjong, and H.-X. Zhou (2016). *Electrostatic effects on the folding stability of FKBP12*. Protein Eng. Des. Sel. **29**, 301-308.
- 224.X. Pang and H.-X. Zhou (2016). *Mechanism and rate constants of the Cdc42 GTPase binding with intrinsically disordered effectors*. Proteins **84**, 674-685.
- 223.J. Guo and H.-X. Zhou (2016). *Protein allostery and conformational dynamics*. Chem. Rev. **116**, 6503-6515.
- 222.A. Wright, P. Batsomboon, J. Dai, I. Hung, H.-X. Zhou, G. Dudley, and T. A. Cross (2016). *Differential binding of rimantadine enantiomers to Influenza A M2 proton channel*. J. Am. Chem. Soc. **138**, 1506-1509.
- 221.Q. Gan, J. Dai, H.-X. Zhou, and L. P. Wollmuth (2016). *The transmembrane domain mediates tetramerization of α -amino-3-hydroxy-5-methyl-4-isoxazolepropionic acid (AMPA) receptors*. J. Biol. Chem. **291**, 6595-6606.
- 220.M. F. Lensink, S. Velankar, A. Kryshchak, S.-Y. Huang, D. Schneidman-Duhovny, A. Sali, J. Segura, N. Fernandez-Fuentes, S. Viswanath, R. Elber, S. Grudinin, P. Popov, E. Neveu, H. Lee, M. Baek, S. Park, L. Heo, G. R. Lee, C. Seok, S. Qin, H.-X. Zhou, D. W. Ritchie, B. Maigret, M.-D. Devignes, A. Ghoorah, M. Torchala, R. A. G. Chaleil, P. A. Bates, E. Ben-Zeev, M. Eisenstein, S. S. Negi, Z. Weng, T. Vreven, B. G. Pierce, T. M. Borrmann, J. Yu, F. Ochsenbein, R. Guerois, A. Vangone, J. P. G. L. M. Rodrigues, G. van Zundert, M. Nellen, L. Xue, E. Karaca, A. S. J. Melquiond, K. Visscher, P. L. Kastiris, A. M. J. J. Bonvin, X. Xu, L. Qiu, C. Yan, J. Li, Z. Ma, J. Cheng, X. Zou, Y. Shen, L. X. Peterson, H.-R. Kim, A. Roy, X. Han, J. Esquivel-Rodriguez, D. Kihara, X. Yu, N. J. Bruce, J. C. Fuller, R. C. Wade, I. Anishchenko, P. J. Kundrotas, I. A. Vakser, K. Imai, K. Yamada, T. Oda, T. Nakamura, K. Tomii, C. Pallara, M. Romero-Durana, B. Jiménez-García, I. H. Moal, J. Fernández-Recio, J. Y. Joung, J. Y. Kim, K. Joo, J. Lee, D. Kozakov, S. Vajda, S. Mottarella, D. R. Hall, D.

- Beglov, A. Mamonov, B. Xia, T. Bohnuud, C. A. Del Carpio, E. Ichiishi, N. Marze, D. Kuroda, S. S. Roy Burman, J. J. Gray, E. Chermak, L. Cavallo, R. Oliva, A. Tovchigrechko, and S. J. Wodak (2016). *Prediction of homo- and hetero-protein complexes by ab-initio and template-based docking: a CASP-CAPRI experiment*. *Proteins* **84** (Suppl 1), 323-348.
219. Y. Miao, R. Fu, H.-X. Zhou, and T. A. Cross (2015). *Dynamic short hydrogen bonds in histidine tetrad of full length M2 proton channel reveal tetrameric structural heterogeneity and functional mechanism*. *Structure* **23**, 2300-2308.
218. X. Pang and H.-X. Zhou (2015). *Disorder-to-order transition of an active-site loop mediates the allosteric activation of sortase A*. *Biophys. J.* **109**, 1706-1715.
217. J. Guo and H.-X. Zhou (2015). *Dynamically driven protein allostery exhibits disparate responses for fast and slow motions*. *Biophys. J.* **108**, 2771-2774.
216. J. Dai, L. P. Wollmuth, and H.-X. Zhou (2015). *Mechanism-based mathematical model for gating of ionotropic glutamate receptors*. *J. Phys. Chem. B* **119**, 10934-10940.
215. N. Das, J. Dai, I. Hung, M. Rajagopalan, H.-X. Zhou, and T. A. Cross (2015). *Structure of CrgA, a cell division structural and regulatory protein from Mycobacterium tuberculosis, in lipid bilayers*. *Proc. Natl. Acad. Sci. USA* **112**, E119-E126.
214. J. Dai and H.-X. Zhou (2015). *Reduced curvature of ligand-binding domain free energy surface underlies partial agonism at NMDA receptors*. *Structure* **23**, 228-236.
213. J. Guo, X. Pang, and H.-X. Zhou (2015). *Two pathways mediate inter-domain allosteric regulation in Pin1*. *Structure* **23**, 237-247.
212. A. Berezhkovskii, A. Szabo, N. Greives, and H.-X. Zhou (2014). *Multidimensional reaction rate theory with anisotropic diffusion*. *J. Chem. Phys.* **141**, 204106.
211. J. Dai and H.-X. Zhou (2014). *General rules for the arrangements and gating motions of pore-lining helices in homomeric ion channels*. *Nat. Commun.* **5**, 4641.
210. N. Greives and H.-X. Zhou (2014). *Both protein dynamics and ligand concentration can shift the binding mechanism between conformational selection and induced fit*. *Proc. Natl. Acad. Sci. USA* **111**, 10197-10202.
209. S. Qin and H.-X. Zhou (2014). *Further development of the FFT-based method for atomistic modeling of protein folding and binding under crowding: optimization of accuracy and speed*. *J. Chem. Theory Comput.* **10**, 2824-2835.
208. R. Kazi, J. Dai, C. Sweeney, H.-X. Zhou, and L. P. Wollmuth (2014). *Mechanical coupling maintains the fidelity of NMDA receptor-mediated currents*. *Nat. Neurosci.* **17**, 914-922.
207. X. Pang and H.-X. Zhou (2014). *Design rules for selective binding of nuclear localization signals to minor site of importin α* . *PLoS ONE* **9**, e91025.
206. H.-X. Zhou and O. Bilsel (2014). *SAXS/SANS probe of intermolecular interactions in concentrated protein solutions*. *Biophys. J.* **106**, 771-773.
205. H.-X. Zhou (2014). *Theoretical frameworks for multiscale modeling and simulation*. *Curr. Opin. Struct. Biol.* **25**, 67-76.
204. X. Pang and H.-X. Zhou (2014). *Distinct mechanisms of a phosphotyrosyl peptide binding to two SH2 domains*. *J. Theor. Comput. Chem.* **13**, 1440003.
203. F. L. Jean-Francoisa, J. Dai, Y. Lue, A. Myrick, E. Rubin, P. G. Fajer, L. Song, H.-X. Zhou, and T. A. Cross (2014). *Binding of MgtR, a Salmonella transmembrane regulatory peptide, to MgtC, a Mycobacterium tuberculosis virulence factor: a structural study*. *J. Mol. Biol.* **426**, 436-446.
202. M. F. Lensink, I. H. Moal, P. A. Bates, P. L. Kastritis, A. S. J. Melquiond, E. Karaca, C. Schmitz, M. van Dijk, A. M. J. J. Bonvin, M. Eisenstein, B. Jimenez-Garcia, S. Grosdidier, A. Solernou, L. Perez-Cano, C. Pallara, J. Fernandez-Recio, J. Xu, P. Muthu, K. P. Kilambi, J. J. Gray, S. Grudin, G. Derevyanko, J. C. Mitchell, J. Wieting, E. Kanamori, Y. Tsuchiya, Y. Murakami, J. Sarmiento, D. M. Standley, M. Shirota, K. Kinoshita, H. Nakamura, M. Chavent, D. W. Ritchie, H. Park, J. Ko, H. Lee, C. Seok, Y. Shen, D. Kozakov, S. Vajda, P. J. Kundrotas, I. A. Vakser, B. G. Pierce, H. Hwang, T. Vreven, Z. Weng, I. Buch, E. Farkash, H. J. Wolfson, M. Zacharias, S. Qin, H.-X. Zhou, S.-Y. Huang, X. Zou, J.

- A. Wojdyla, C. Kleanthous, and S. J. Wodak (2014). *Blind prediction of interfacial water positions in CAPRI*. *Proteins* **82**, 620-632.
- 201.S. Qin and H.-X. Zhou (2013). *Effects of macromolecular crowding on the conformational ensembles of disordered proteins*. *J. Phys. Chem. Lett.* **4**, 3429–3434.
- 200.G. Heymann, J. Dai, M. Li, S. D. Silberberg, H.-X. Zhou, and K. J. Swartz (2013). *Inter- and intrasubunit interactions between transmembrane helices in the open state of P2X receptor channels*. *Proc. Natl. Acad. Sci. USA* **110**, E4045-E4054.
- 199.A. R. Cormier, X. Pang, M. I. Zimmerman, H.-X. Zhou, and A. K. Paravastu (2013). *Molecular structure of RADA16-I designer self-assembling peptide nanofibers*. *ACS Nano* **7**, 7562-7572.
- 198.S. Qin and H.-X. Zhou (2013). *FFT-based method for modeling protein folding and binding under crowding: benchmarking on ellipsoidal and all-atom crowders*. *J. Chem. Theory Comput.* **9**, 4633-4643.
- 197.A. C. Miklos, M. Sumpter, and H.-X. Zhou (2013). *Competitive interactions of ligands and macromolecular crowders with maltose binding protein*. *PLoS ONE* **8**, e74969.
- 196.S. Qin and H.-X. Zhou (2013). *Using the concept of transient complex for affinity predictions in CAPRI rounds 20-27 and beyond*. *Proteins* **81**, 2229-2236.
- 195.R. Moretti, S. J. Fleishman, R. Agius, M. Torchala, P. A. Bates, P. L. Kastritis, J. P. G. L. M. Rodrigues, M. Trellet, A. M. J. J. Bonvin, M. Cui, M. Rومان, D. Gillis, Y. Dehouck, I. Moal, M. Romero-Durana, L. Perez-Cano, C. Pallara, B. Jimenez, J. Fernandez-Recio, S. Flores, M. Pacella, K. P. Kilambi, J. J. Gray, P. Popov, S. Grudin, J. Esquivel-Rodriguez, D. Kihara, N. Zhao, D. Korkin, X. Zhu, O. N. A. Demerdash, J. C. Mitchell, E. Kanamori, Y. Tsuchiya, H. Nakamura, H. Lee, H. Park, C. Seok, J. Sarmiento, S. Liang, S. Teraguchi, D. M. Standley, H. Shimoyama, G. Terashi, M. Takeda-Shitaka, M. Iwadate, H. Umeyama, D. Beglov, D. R. Hall, D. Kozakov, S. Vajda, B. G. Pierce, H. Hwang, T. Vreven, Z. Weng, Y. Huang, H. Li, X. Yang, X. Ji, S. Liu, Y. Xiao, M. Zacharias, S. Qin, H.-X. Zhou, S.-Y. Huang, X. Zou, S. Velankar, J. Janin, S. J. Wodak, and D. Baker (2013). *Community-wide evaluation of methods for predicting the effect of mutations on protein-protein interactions*. *Proteins* **81**, 1980-1987.
- 194.X. Pang and H.-X. Zhou (2013). *Activation of signaling receptors: do ligands bind to receptor monomer, dimer, or both?* *BMC Biophys.* **6**, 7.
- 193.H.-X. Zhou and P. A. Bates (2013). *Modeling protein association mechanisms and kinetics*. *Curr. Opin. Struct. Biol.* **23**, 887-293.
- 192.S. R. Leonard, A. R. Cormier, X. Pang, M. I. Zimmerman, H.-X. Zhou, and A. K. Paravastu (2013). *Solid-state NMR evidence for β -hairpin structure within MAX8 designer peptide nanofibers*. *Biophys. J.* **105**, 222-230.
- 191.H. Dong, M. Yi, T.A. Cross, and H.-X. Zhou (2013). *Ab initio calculations and validation of the pH-dependent structures of the His37-Trp41 quartet, the heart of acid activation and proton conductance in the M2 protein of Influenza A virus*. *Chem. Sci.* **4**, 2776-2787.
- 190.J. Dai and H.-X. Zhou (2013). *An NMDA receptor gating mechanism developed from MD simulations reveals molecular details underlying subunit-specific contributions*. *Biophys. J.* **104**, 2170-2181.
- 189.H.-X. Zhou and T. A. Cross (2013). *Modeling the membrane environment has implications for membrane protein structure and function: Influenza A M2 protein*. *Protein Sci.* **22**, 381-394.
- 188.H.-X. Zhou (2013). *Influences of crowded cellular environments on protein folding, binding, and oligomerization: biological consequences and potentials of atomistic modeling*. *FEBS. Lett.* **587**, 1053-1061.
- 187.S. Qin, J. Mittal, and H.-X. Zhou (2013). *Folding free energy surfaces of three small proteins under crowding: validation of the postprocessing method by direct simulation*. *Phys. Biol.* **10**, 045001.
- 186.H.-X. Zhou (2013). *Polymer crowders and protein crowders act similarly on protein folding stability*. *FEBS. Lett.* **587**, 394-397.
- 185.H.-X. Zhou and S. Qin (2013). *Simulation and modeling of crowding effects on the thermodynamic and kinetic properties of proteins with atomic details*. *Biophys. Rev.* **5**, 207-215.
- 184.H.-X. Zhou and T. A. Cross (2013). *Influences of membrane mimetic environments on membrane protein structures*. *Annu. Rev. Biophys.* **42**, 361-392.

- 183.S. Qin and H.-X. Zhou (2013). *PPPE: a suite of web servers for predictions ranging from protein structure to binding kinetics*. Biophys. Rev. **5**, 41-46.
- 182.X. Pang and H.-X. Zhou (2013). *Poisson-Boltzmann calculations: van der Waals or molecular surface?* Commun. Comput. Phys. **13**, 1-12.
- 181.S. Qin, L. Cai, and H.-X. Zhou (2012). *A method for computing association rate constants of atomistically represented proteins under macromolecular crowding*. Phys. Biol. **9**, 066008.
- 180.N. Greives and H.-X. Zhou (2012). *BDflex: a method for efficient treatment of molecular flexibility in calculating protein-ligand binding rate constants from Brownian dynamics simulations*. J. Chem. Phys. **137**, 135105.
- 179.C. K. P. Long, H.-X. Zhou, and P. B. Chase (2012). *Familial hypertrophic cardiomyopathy related E180G mutation increases flexibility of human cardiac α -tropomyosin*. FEBS Lett. **586**, 3503-3507.
- 178.Y. Phillip, M. Harel, R. Khait, S. Qin, H.-X. Zhou, and G. Schreiber (2012). *Contrasting factors on the kinetic path to protein complex formation nullify the effects of crowding agents*. Biophys. J. **103**, 1011-1019.
- 177.X. Pang, K. H. Zhou, S. Qin, and H.-X. Zhou (2012). *Prediction and dissection of widely-varying association rate constants of actin-binding proteins*. PLoS Comput. Biol. **8**, e1002696.
176. H.-X. Zhou, X. Pang, and L. Cai (2012). *Rate constants and mechanisms of intrinsically disordered proteins binding to structured targets*. Phys. Chem. Chem. Phys. **14**, 10466-10476.
- 175.J. Du, T. A. Cross, and H.-X. Zhou (2012). *Recent progress in structure-based anti-influenza drug design*. Drug Discov. Today **11**, 1111-1120.
- 174.J. Du, H. Dong, and H.-X. Zhou (2012). *Size matters in activation/inhibition of ligand-gated ion channels*. Trends Pharmacol. Sci. **33**, 482-493.
- 173.C. K. P. Long, H.-X. Zhou, and P. B. Chase (2012). *Persistence length of human cardiac α -tropomyosin measured by single molecule direct probe microscopy*. PLoS ONE **7**, e39676.
- 172.H. Dong, M. Sharma, H.-X. Zhou, and T. A. Cross (2012). *Glycines: role in α -helical membrane protein structures and a potential indicator for native conformation*. Biochemistry **51**, 4779-4789.
- 171.J. Du, H. Dong, and H.-X. Zhou (2012). *Gating mechanism of a P2X4 receptor developed from normal mode analysis and molecular dynamics simulations*. Proc. Natl. Acad. Sci. USA. **109**, 4140-4145.
- 170.X. Pang and H.-X. Zhou (2012). *A common model for cytokine receptor activation: combined scissor-like rotation and self-rotation of receptor dimer induced by class I cytokine*. PLoS Comput. Biol. **8**, e1002427.
- 169.T. A. Cross, H. Dong, M. Sharma, D. D. Busath, and H.-X. Zhou (2012). *M2 protein from influenza A: from multiple structures to biophysical and functional insights*. Curr. Opin. Virol. **2**, 128-133.
- 168.A. Szabo and H.-X. Zhou (2012). *Role of diffusion in the kinetics of reversible enzyme-catalyzed reactions*. Bull. Korean Chem. Soc. **33**, 925-928.
- 167.H.-X. Zhou (2012). *Intrinsic disorder: signaling via highly specific but short-lived association*. Trends Biochem. Sci. **37**, 43-48.
- 166.S. Qin, X. Pang, and H.-X. Zhou (2011). *Automated prediction of protein association rate constants*. Structure **19**, 1744-1751.
- 165.H.-X. Zhou (2011). *Mechanistic insight into the H₂O/D₂O isotope effect in the proton transport of the Influenza virus M2 protein*. J. Membr. Biol. **244**, 93-96.
- 164.J. L. Barreda and H.-X. Zhou (2011). *Theory and simulation of diffusion-influenced, stochastically gated ligand binding to buried sites*. J. Chem. Phys. **135**, 145101.
- 163.S. J. Fleishman, T. A. Whitehead, E.-M. Strauch, J. E. Corn, S. Qin, H.-X. Zhou, ..., and D. Baker (2011). *Community-wide assessment of protein-interface modeling suggests improvements to design methodology*. J. Mol. Biol. **414**, 289-302.
- 162.A. M. Berezhkovskii, A. Szabo, and H.-X. Zhou (2011). *Diffusion-influenced ligand binding to buried sites in macromolecules and transmembrane channels*. J. Chem. Phys. **135**, 075103.
- 161.X. Pang, S. Qin, and H.-X. Zhou (2011). *Rationalizing 5,000-fold differences in receptor-binding rate constants of four cytokines*. Biophys. J. **101**, 1175-1183.

- 160.H. Dong and H.-X. Zhou (2011). *Atomistic mechanism for the activation and desensitization of an AMPA-subtype glutamate receptor*. Nat. Commun. **2**, 354.
- 159.H.-X. Zhou (2011). *Speedup of the search for specific sites on DNA by conformational switch of nonspecifically bound proteins*. Proc. Natl. Acad. Sci. USA. **108**, 8651-8656.
- 158.H.-X. Zhou (2011). *Equivalence of two approaches for modeling ion permeation through a transmembrane channel with an internal binding site*. J. Chem. Phys. **134**, 135101.
- 157.H.-X. Zhou (2011). *Q&A: What is biophysics?* BMC Biology **9**, 13.
- 156.J. L. Barreda and H.-X. Zhou (2011). *A solvable model for the diffusion and reaction of neurotransmitters in a synaptic junction*. BMC Biophys. **4**, 5.
- 155.L. Cai and H.-X. Zhou (2011). *Theory and simulation on the kinetics of protein-ligand binding coupled to conformational change*. J. Chem. Phys. **134**, 105101.
- 154.H.-X. Zhou (2011). *A theory for the proton transport of the influenza virus M2 protein: extensive test against conductance data*. Biophys. J. **100**, 912-921.
- 153.S. Qin and H.-X. Zhou (2011). *Structural models of protein-DNA complexes based on interface prediction and docking*. Curr. Protein Pept. Sci. **12**, 531-539.
- 152.T. A. Cross, M. Sharma, M. Yi, and H.-X. Zhou (2011). *Influence of solubilizing environments on membrane protein structures*. Trends Biochem. Sci. **36**, 117-125.
- 151.M. Sharma, C. Li, D. D. Busath, H.-X. Zhou, and T. A. Cross (2011). *Drug sensitivity, drug-resistant mutations, and structures of three conductance domains of viral porins*. BBA-Biomembranes **1808**, 538-546.
- 150.W. Lee, X. Zeng, H.-X. Zhou, V. Bennett, W. Yang, and P. E. Marszalek (2010). *Full reconstruction of a vectorial protein folding pathway by atomic force microscopy and molecular dynamics simulations*. J. Biol. Chem. **285**, 38167-38172.
- 149.M. Sharma, M. Yi, H. Dong, H. Qin, E. Peterson, D. D. Busath, H.-X. Zhou, and T. A. Cross (2010). *Insight into the mechanism of the influenza A proton channel from a structure in a lipid bilayer*. Science **330**, 509-512.
- 148.H.-X. Zhou, *Speeding up in a crowd*. Physics **3**, 77.
- 147.H.-X. Zhou (2010). *Diffusion-influenced transport of ions across a transmembrane channel with an internal binding site*. J. Phys. Chem. Lett. **1**, 1973-1976.
- 146.H. Dong, S. Qin, and H.-X. Zhou (2010). *Effects of macromolecular crowding on protein conformational changes*. PLOS Comput. Biol. **6**, e1000833.
- 145.S. Qin and H.-X. Zhou (2010). *Selection of near-native poses in CAPRI rounds 13-19*. Proteins **78**, 3166-3173.
- 144.H.-X. Zhou (2010). *Rate theories for biologists*. Q. Rev. Biophys. **43**, 219-293.
- 143.H. Tjong and H.-X. Zhou (2010). *The folding transition-state ensemble of a four-helix bundle protein: helix propensity as a determinant and macromolecular crowding as a probe*. Biophys. J. **98**, 2273-2280.
- 142.S. Qin and H.-X. Zhou (2010). *Generalized fundamental measure theory for atomistic modeling of macromolecular crowding*. Phys. Rev. E **81**, 031919.
- 141.H.-X. Zhou (2010). *From induced fit to conformational selection: a continuum of binding mechanism controlled by the timescale of conformational transitions*. Biophys. J. **98**, L15-L17.
- 140.S. Qin, D. D. L. Minh, J. A. McCammon, and H.-X. Zhou (2010). *Method to predict crowding effects by postprocessing molecular dynamics trajectories: application to the flap dynamics of HIV-1 protease*. J. Phys. Chem. Lett. **1**, 107-110.
- 139.H.-X. Zhou and J. A. McCammon (2010). *The gates of ion channels and enzymes*. Trends Biochem. Sci. **35**, 179-185.
- 138.X. Zeng, H. Hu, H.-X. Zhou, P. E. Marszalek, and W. Yang (2010). *Equilibrium sampling for biomolecules under mechanical tension*. Biophys. J. **98**, 733-740.
- 137.A. Bazavov, B. A. Berg, and H.-X. Zhou (2010). *Application of biased metropolis algorithms: from protons to proteins*. Math. Comput. Simul. **80**, 1056-1067.

136. A. W. Maniccia, W. Yang, J. A. Johnson, S. Li, H. Tjong, H.-X. Zhou, L. A. Shaket, and J. J. Yang (2009). *Inverse tuning of metal binding affinity and protein stability by altering charged coordination residues in designed calcium binding proteins*. *PMC Biophysics* **2**, 11.
135. M. Yi, T. A. Cross, and H.-X. Zhou (2009). *Conformational heterogeneity of the M2 proton channel and a structural model for channel activation*. *Proc. Natl. Acad. Sci. USA* **106**, 13311-13316.
134. J. Batra, K. Xu, S. Qin, and H.-X. Zhou (2009). *Effect of macromolecular crowding on protein binding stability: modest stabilization and significant biological consequences*. *Biophys. J.* **97**, 906-911.
133. S. Qin and H.-X. Zhou (2009). *Atomistic modeling of macromolecular crowding predicts modest increases in protein folding and binding stability*. *Biophys. J.* **97**, 12-19.
132. S. Qin and H.-X. Zhou (2009). *Dissection of the high rate constant for the binding of a ribotoxin to the ribosome*. *Proc. Natl. Acad. Sci. USA*. **106**, 6974-7979.
131. H.-X. Zhou and M. K. Gilson (2009). *Theory of free energy and entropy in noncovalent binding*. *Chem. Rev.* **109**, 4092-4107.
130. J. Batra, K. Xu, and H.-X. Zhou (2009). *Nonadditive effects of mixed crowding on protein stability*. *Proteins* **77**, 133-138.
129. H.-X. Zhou (2009). *Crowding effects of membrane proteins*. *J. Phys. Chem. B* **113**, 7995-8005.
128. G. Schreiber, G. Haran, and H.-X. Zhou (2009). *Fundamental aspects of protein-protein association kinetics*. *Chem. Rev.* **109**, 839-860.
127. G.-C. Dong, P.-H. Chuang, K.-c. Chang, P.-s. Jan, P.-I. Hwang, H.-B. Wu, M. Yi, H.-X. Zhou, and H. M. Chen (2009). *Blocking effect of an immuno-suppressive agent, cynarin, on CD28 of T-Cell receptor*. *Pharm. Res.* **26**, 375-381.
126. J.-M. Yuan, C.-L. Chyan, H.-X. Zhou, T.-Y. Chung, H. Peng, G. Ping, and G. Yang (2008). *The effects of macromolecular crowding on the mechanical stability of protein molecules*. *Protein Sci.* **17**, 2156-2166.
125. S. Li, W. Yang, A. W. Maniccia, D. Barrow Jr., H. Tjong, H.-X. Zhou, and J. J. Yang (2008). *Rational design of a conformation switchable Ca^{2+} and Tb^{3+} binding protein without using multiple coupled metal binding sites*. *FEBS J.* **275**, 5048-5061.
124. H.-X. Zhou (2008). *The debut of PMC Biophysics*. *PMC Biophysics* **1**, 1.
123. H. Tjong and H.-X. Zhou (2008). *Accurate calculations of binding, folding, and transfer free energies by a scaled generalized Born method*. *J. Chem. Theory Comput.* **4**, 1733-1744.
122. M. Yi, H. Nymeyer, and H.-X. Zhou (2008). *Test of the Gouy-Chapman theory for a charged lipid membrane against explicit-solvent molecular dynamics simulations*. *Phys. Rev. Lett.* **101**, 038103.
121. M. Yi, T. A. Cross, and H.-X. Zhou (2008). *A secondary gate as a mechanism for inhibition of the M2 proton channel by amantadine*. *J. Phys. Chem. B* **112**, 7977-7979.
120. H.-X. Zhou (2008). *A minimum-reaction-flux solution to master-equation models of protein folding*. *J. Chem. Phys.* **128**, 195104.
119. H.-X. Zhou, S. Qin, and H. Tjong (2008). *Modeling protein-protein and protein-nucleic acid interactions: structure, thermodynamics, and kinetics*. *Annu. Report Comput. Chem.* **4**, 67-87.
118. H.-X. Zhou (2008). *Effect of mixed macromolecular crowding agents on protein folding*. *Proteins* **72**, 1109-1113.
117. M. Yi, H. Tjong, and H.-X. Zhou (2008). *Spontaneous conformational change and toxin binding in $\alpha 7$ acetylcholine receptor: insight into channel activation and inhibition*. *Proc. Natl. Acad. Sci. USA* **105**, 8280-8285.
116. H. Tjong and H.-X. Zhou (2008). *Prediction of protein solubility from calculation of transfer free energy*. *Biophys. J.* **95**, 2601-2609.
115. R. Alsallaq and H.-X. Zhou (2008). *Protein association with circular DNA: rate enhancement by nonspecific binding*. *J. Chem. Phys.* **128**, 115108.
114. H. Tjong and H.-X. Zhou (2008). *On the dielectric boundary in Poisson-Boltzmann calculations*. *J. Chem. Theory Comput.* **4**, 507-514.

113. H.-X. Zhou, G. Rivas, and A. P. Minton (2008). *Macromolecular crowding and confinement: biochemical, biophysical, and potential physiological consequences*. *Annu. Rev. Biophys.* **37**, 375-397.
112. H.-X. Zhou (2008). *Calculation of free-energy differences and potentials of mean force by a multi-energy gap method*. *J. Chem. Phys.* **128**, 114104.
111. C. Li, M. Yi, J. Hu, H.-X. Zhou, and T. A. Cross (2008). *Solid-state NMR and MD simulations of the anti-viral drug amantadine solubilized in DMPC bilayers*. *Biophys. J.* **94**, 1295-1302.
110. H. Nymeyer and H.-X. Zhou (2008). *A Method to determine dielectric constants in non-homogeneous systems: application to biological membranes*. *Biophys. J.* **94**, 1185-1193.
109. W. Yang, H. Nymeyer, H.-X. Zhou, B. Berg, and R. Bruschweiler (2008). *Quantitative computer simulations of biomolecules: a snapshot*. *J. Comput. Chem.* **29**, 668-672.
108. R. Alsallaq and H.-X. Zhou (2008). *Electrostatic rate enhancement and transient complex of protein-protein association*. *Proteins* **71**, 320-335.
107. S. Qin and H.-X. Zhou (2008). *Prediction of salt and mutational effects on the association rate of U1A protein and U1 small nuclear RNA stem/loop II*. *J. Phys. Chem. B* **112**, 5955-5960.
106. H.-X. Zhou (2008). *Protein folding in confined and crowded environments*. *Arch. Biochem. Biophys.* **469**, 76-82.
105. H.-X. Zhou (2007). *Helix formation inside a nanotube: possible influence of backbone-water hydrogen bonding by the confining surface through modulation of water activity*. *J. Chem. Phys.* **127**, 245101.
104. N. Bhattacharya, M. Yi, H.-X. Zhou, and T. Logan (2007). *Backbone dynamics in an intramolecular prolylpeptide-SH3 complex from the diphtheria toxin repressor, DtxR*. *J. Mol. Biol.* **374**, 977-992.
103. S. Qin and H.-X. Zhou (2007). *A holistic approach to protein docking*. *Proteins* **69**, 743-749.
102. S. Qin and H.-X. Zhou (2007). *meta-PPISP: a meta web server for protein-protein interaction site prediction*. *Bioinformatics* **22**, 3386-3387.
101. H.-X. Zhou and S. Qin (2007). *Interaction-site prediction for protein complexes: a critical assessment*. *Bioinformatics* **22**, 2203-2209.
100. H. Tjong and H.-X. Zhou (2007). *GBr⁶NL: a generalized Born method for accurately reproducing solvation energy of the nonlinear Poisson-Boltzmann equation*. *J. Chem. Phys.* **126**, 195102.
99. H. Tjong, S. Qin, and H.-X. Zhou (2007). *PI²PE: protein interface/interior prediction engine*. *Nucl. Acids Res.* **35**, W357-W362.
98. S. Qin and H.-X. Zhou (2007). *Do electrostatic interactions destabilize protein-nucleic acid binding?* *Biopolymers* **86**, 112-118.
97. H. Tjong and H.-X. Zhou (2007). *GBr⁶: a parameterization-free, accurate, analytical generalized Born method*. *J. Phys. Chem. B* **111**, 3055-3061.
96. R. Alsallaq and H.-X. Zhou (2007). *Prediction of protein-protein association rates from a transition-state theory*. *Structure* **15**, 215-224.
95. H. Tjong and H.-X. Zhou (2007). *DISPLAR: an accurate method for predicting DNA-binding sites on protein surfaces*. *Nucl. Acids Res.* **35**, 1465-1477.
94. M. K. Gilson and H.-X. Zhou (2007). *Calculation of protein-ligand binding affinities*. *Annu. Rev. Biophys. Biomol. Struct.* **36**, 21-42.
93. R. Alsallaq and H.-X. Zhou (2007). *Energy landscape and transition state of protein-protein association*. *Biophys. J.* **92**, 1486-1502.
92. H. Tjong and H.-X. Zhou (2006). *The dependence of electrostatic solvation energy on dielectric constants in Poisson-Boltzmann calculations*. *J. Chem. Phys.* **125**, 206101.
91. H.-X. Zhou (2006). *Quantitative relation between intermolecular and intramolecular binding of pro-rich peptides to SH3 domains*. *Biophys. J.* **91**, 3170-3181.
90. X. Huang and H.-X. Zhou (2006). *Similarity and difference in the unfolding of thermophilic and mesophilic cold shock proteins studied by molecular dynamics simulations*. *Biophys. J.* **91**, 2451-2463.
89. F. Dong and H.-X. Zhou (2006). *Electrostatic contribution to the binding stability of protein-protein complexes*. *Proteins* **65**, 87-102.

88. J. Hu, R. Fu, K. Nishimura, L. Zhang, H.-X. Zhou, D. D. Busath, V. Vijayvergiya, and T. A. Cross (2006). *Histidines, heart of the hydrogen ion channel from influenza A virus: toward an understanding of conductance and proton selectivity*. Proc. Natl. Acad. Sci. USA **103**, 6865-6870.
87. H.-X. Zhou (2005). *How do biomolecular systems speed up and regulate rates?* Phys. Biol. **2**, R1-R25.
86. B. Berg and H.-X. Zhou (2005). *Rugged Metropolis sampling with simultaneous updating of two dynamical variables*. Phys. Rev. E **72**, 016712.
85. H. Chen and H.-X. Zhou (2005). *Prediction of solvent accessibility and sites of deleterious mutations from protein sequence*. Nucl. Acids Res. **33**, 3193-3199.
84. D. S. Spencer, K. Xu, T. M. Logan, and H.-X. Zhou (2005). *Effects of pH, salt, and macromolecular crowding on the stability of FK506-binding protein: an integrated experimental and theoretical study*. J. Mol. Biol. **351**, 219-232.
83. A. D. J. van Dijk, S. J. de Vries, C. Dominguez, H. Chen, H.-X. Zhou, and A. M. J. J. Bonvin (2005). *Data-driven docking: HADDOCK's adventures in CAPRI*. Proteins **60**, 232-238.
82. H. Chen and H.-X. Zhou (2005). *Prediction of interface residues in protein-protein complexes by a consensus neural network method: test against NMR data*. Proteins **61**, 21-35.
81. H.-X. Zhou (2005). *Interactions of macromolecules with salt ions: an electrostatic theory for the Hofmeister effect*. Proteins **61**, 69-78.
80. X. Huang, F. Dong, and H.-X. Zhou (2005). *Electrostatic recognition and induced fit in the κ -PVIIA toxin binding to Shaker potassium channel*. J. Am. Chem. Soc **127**, 6836-6849.
79. H.-X. Zhou (2005), *A model for the mediation of processivity of DNA-targeting proteins by nonspecific binding: dependence on DNA length and presence of obstacles*. Biophys. J. **88**, 1608-1615.
78. H.-X. Zhou and A. Szabo (2004), *Enhancement of association rates by nonspecific binding to DNA and cell membranes*. Phys. Rev. Lett. **93**, 178101.
77. H.-X. Zhou (2004), *Polymer models of protein stability, folding, and interactions*. Biochemistry. **43**, 2141-2154.
76. H.-X. Zhou (2004), *Loops, linkages, rings, catenanes, cages, and crowders: entropy-based strategies for stabilizing proteins*. Acc. Chem. Res. **37**, 123-130.
75. H.-X. Zhou (2004), *Protein folding and binding in confined spaces and in crowded solutions*. J. Mol. Recog. **17**, 368-375.
74. H.-X. Zhou (2004), *Improving the understanding of human genetic diseases through predictions of protein structures and protein-protein interaction sites*. Curr. Med. Chem. **11**, 539-549.
73. H.-X. Zhou (2003), *How often does the myristoylated N-terminal latch of c-Abl come off?* FEBS Lett. **552**, 160-162.
72. H.-X. Zhou (2003), *Effect of backbone cyclization on protein folding stability: chain entropies of both the unfolded and the folded states are restricted*. J. Mol. Biol. **332**, 257-264.
71. H.-X. Zhou (2003), *Association and dissociation kinetics of colicin E3 and immunity protein 3: convergence of theory and experiment*. Protein Sci. **12**, 2379-2382.
70. H.-X. Zhou (2003), *Effect of catenation on protein folding stability*. J. Am. Chem. Soc. **125**, 9280-9281.
69. H.-X. Zhou (2003), *Quantitative account of the enhanced affinity of two linked scFvs specific for different epitopes on the same antigen*. J. Mol. Biol. **329**, 1-8.
68. F. Dong, M. Vijayakumar, and H.-X. Zhou (2003), *Comparison of calculation and experiment implicates significant electrostatic contributions to the binding stability of barnase and barstar*. Biophys. J. **85**, 49-60.
67. H.-X. Zhou (2003), *Direct test of the Gaussian-chain model for treating residual charge-charge interactions in the unfolded state of proteins*. J. Am. Chem. Soc. **125**, 2060-2061.
66. H.-X. Zhou and F. Dong (2003), *Electrostatic contributions to the stability of a thermophilic cold shock protein*. Biophys. J. **84**, 2216-2222.
65. H.-X. Zhou (2003), *Theory for the rate of contact formation in a polymer chain with local conformational transitions*. J. Chem. Phys. **118**, 2010-2015.

64. H.-X. Zhou (2002), *Toward the physical basis of thermophilic proteins: linking of enriched polar interactions and reduced heat capacity of unfolding*. *Biophys. J.* **83**, 3126-3133.
63. H.-X. Zhou (2002), *Residual charge interactions in unfolded staphylococcal nuclease can be explained by the Gaussian-chain model*. *Biophys. J.* **83**, 2981-2986.
62. F. Dong and H.-X. Zhou (2002), *Electrostatic contributions to T4 lysozyme stability: solvent-exposed charges versus semi-buried salt bridges*. *Biophys. J.* **83**, 1341-1347.
61. H.-X. Zhou (2002), *Residual electrostatic effects in the unfolded state of the N-terminal domain of L9 can be attributed to non-specific non-local charge-charge interactions*. *Biochemistry* **41**:6533-6538.
60. H.-X. Zhou (2002), *Dimensions of denatured proteins chains from hydrodynamic data*. *J. Phys. Chem. B.* **106**, 5769-5775.
59. H.-X. Zhou (2002), *A Gaussian-chain model for treating residual charge-charge interactions in the unfolded state of proteins*. *Proc. Natl. Acad. Sci. USA* **99**, 3569-3574.
58. H.-X. Zhou and R. Zwanzig (2002), *Barrier crossing coupled to a small set of oscillators*. *J. Phys. Chem. A* **106**, 7562-7564.
57. A. H. Boschitsch, M. O. Fenley, and H.-X. Zhou (2002), *Fast boundary element method for the linear Poisson-Boltzmann equation*. *J. Phys. Chem. B.* **202**, 2741-2754.
56. H.-X. Zhou (2002), *A model for the binding of the inactivation N-terminal to the ion pore of Shaker potassium channel: both electrostatic attraction and covalent linkage are required for rapid inactivation*. *J. Phys. Chem. B* **202**, 2393-2397.
55. H.-X. Zhou (2001), *The affinity-enhancing roles of flexible linkers in two-domain DNA-binding proteins*. *Biochemistry* **40**, 15069-15073.
54. H.-X. Zhou and K. A. Dill (2001), *Stabilization of proteins in confined spaces*. *Biochemistry* **40**, 11289-11293.
53. M. Vijayakumar and H.-X. Zhou (2001), *Salt bridges stabilize the folded structure of barnase*. *J. Phys. Chem. B* **105**, 7334-7340.
52. H.-X. Zhou (2001), *Single-chain versus dimeric protein folding: thermodynamic and kinetic consequences of covalent linkage*. *J. Am. Chem. Soc.* **123**, 6730-6731.
51. H.-X. Zhou (2001), *Loops in proteins can be modeled as worm-like chains*. *J. Phys. Chem. B* **105**, 6763-6766.
50. H.-X. Zhou and Y. Shan (2001), *Prediction of protein interaction sites from sequence profiles and residue neighbor list*. *Proteins* **44**, 336-343.
49. H.-X. Zhou (2001), *Disparate ionic-strength dependence of on and off rates in protein-protein association*. *Biopolymers* **59**, 427-433.
48. H.-X. Zhou and G. Wang (2001), *Predicted structures of two proteins involved in human diseases*. *Cell Biochem. Biophys.* **35**, 35-47.
47. H.-X. Zhou (2001), *A unified picture of protein hydration: prediction of hydrodynamic properties from known structures*. *Biophys. Chem.* **93**, 171-179.
46. Y. Shan, G. Wang, and H.-X. Zhou (2001), *Fold recognition and accurate query-template alignment by a combination of PSI-BLAST and threading*. *Proteins* **42**, 23-37.
45. M. Vijayakumar and H.-X. Zhou (2000), *Prediction of residue-residue pair frequencies in proteins*. *J. Phys. Chem. B* **104**, 9755-9764.
44. Y. Shan and H.-X. Zhou (2000), *Correspondence of potentials of mean force in proteins and in liquids*. *J. Chem. Phys.* **113**, 4794-4798.
43. A. M. Berezhkovskii, A. Szabo, G. H. Weiss, and H.-X. Zhou (1999), *Reaction dynamics on a thermally fluctuating potential*. *J. Chem. Phys.* **111**, 9952-9957.
42. M. Vijayakumar, H. Qian, and H.-X. Zhou (1999), *Hydrogen bonds between short polar side chains and peptide backbone: prevalence in proteins and effects on helix-forming propensities*. *Proteins* **34**, 497-507.
41. H.-X. Zhou, S. T. Wlodek, and J. A. McCammon (1998), *Conformation gating as a mechanism for enzyme specificity*. *Proc. Natl. Acad. Sci. USA* **95**, 9280-9283.

40. M. Vijayakumar, K.-Y. Wong, G. Schreiber, A. R. Fersht, A. Szabo, and H.-X. Zhou (1998), *Electrostatic enhancement of diffusion-controlled protein-protein association: comparison of theory and experiment on barnase and barstar*. J. Mol. Biol. **278**, 1015-1024.
39. H.-X. Zhou (1998), *Theory of the diffusion-influenced substrate binding rate to a buried and gated active site*. J. Chem. Phys. **108**, 8146-8154.
38. H.-X. Zhou (1998), *Comparison of three Brownian-dynamics algorithms for calculating rate constants of diffusion-influenced reactions*. J. Chem. Phys. **108**, 8139-8145.
37. H.-X. Zhou, J. M. Briggs, S. Tara, and J. A. McCammon (1998), *Correlation between rate of enzyme-substrate diffusional encounter and average Boltzmann factor around active site*. Biopolymers **45**, 355-360.
36. H.-X. Zhou (1997), *Enhancement of protein-protein association rate by interaction potential: accuracy of prediction based on local Boltzmann factor*. Biophys. J. **73**, 2441-2445.
35. H.-X. Zhou, K.-Y. Wong, and M. Vijayakumar (1997), *Design of fast enzymes by optimizing interaction potential in active site*. Proc. Natl. Acad. Sci. USA **94**, 12372-12377.
34. H.-X. Zhou (1997), *Theory and simulation of the influence of diffusion in enzyme-catalyzed reactions*. J. Phys. Chem. B **101**, 6642-6651.
33. H.-X. Zhou and M. Vijayakumar (1997), *Modeling of protein conformational fluctuations in pKa predictions*. J. Mol. Biol. **267**, 1002-1011.
32. H.-X. Zhou (1997), *Control of reduction potential by protein matrix: lesson from a spherical protein model*. J. Biol. Inorg. Chem. **2**, 109-113.
31. H.-X. Zhou, J. M. Briggs, and J. A. McCammon (1996), *A 240-fold electrostatic rate-enhancement for acetylcholinesterase-substrate binding can be predicted by the potential within the active site*. J. Am. Chem. Soc. **118**, 13069-13070.
30. H.-X. Zhou (1996), *Effect of interaction potentials in diffusion-influenced reactions with small reactive regions*. J. Chem. Phys. **105**, 7235-7237.
29. H.-X. Zhou and A. Szabo (1996), *Theory and simulation of the time-dependent rate coefficients of diffusion-influenced reactions*. Biophys. J. **71**, 2440-2457.
28. H.-X. Zhou (1996), *Dielectric continuum model for calculating reorganization free energies of electron transfer in proteins*. J. Chem. Phys. **105**, 3726-3733.
27. H.-X. Zhou and Y. Chen (1996), *Chemically driven motility of Brownian particles*. Phys. Rev. Lett. **77**, 194-197.
26. M. J. Potter, B. Luty, H.-X. Zhou, and J. A. McCammon (1996), *Time-dependent rate coefficients from Brownian dynamics simulations*. J. Phys. Chem. **100**, 5149-5154.
25. H.-X. Zhou and A. Szabo (1996), *Theory and simulation of stochastically-gated diffusion-influenced reactions*. J. Phys. Chem. **100**, 2597-2604.
24. J. A. Ernst, R. T. Clubb, H.-X. Zhou, A. M. Gronenborn, and G. M. Clore (1995), *Use of NMR to detect water within nonpolar protein cavities*. Science **270**, 1848-1849.
23. H.-X. Zhou (1995), *Calculation of translational friction and intrinsic viscosity. II. Application to globular proteins*. Biophys. J. **69**, 2298-2303.
22. H.-X. Zhou (1995), *Calculation of translational friction and intrinsic viscosity. I. General formulation for arbitrarily shaped particles*. Biophys. J. **69**, 2286-2297.
21. H.-X. Zhou and A. Szabo (1995), *Microscopic formulation of Marcus' theory of electron transfer*. J. Chem. Phys. **103**, 3481-3494.
20. J. A. Ernst, R. T. Clubb, H.-X. Zhou, A. M. Gronenborn, and G. M. Clore (1995), *Demonstration of positionally disordered water within a protein hydrophobic cavity by NMR*. Science **267**, 1813-1817.
19. H.-X. Zhou (1995), *Continuum-model studies of redox reactions, complex formation, and electron transfer: the paradigm of cytochrome c and cytochrome c peroxidase*, in A. Pullman, J. Jortner, and B. Pullman (Eds.), "Modelling of Biomolecular Structures and Mechanisms", 381-398, Kluwer Academic Publishers, Dordrecht.

18. H.-X. Zhou (1994), *Effects of mutations and complex formation on the redox potentials of cytochrome c and cytochrome c peroxidase*. J. Am. Chem. Soc. **116**, 10362-10375.
17. J. F. Douglas, H.-X. Zhou, and J. B. Hubbard (1994), *Hydrodynamic friction and the electrostatic capacitance of an arbitrarily-shaped objects*. Phys. Rev. E **49**, 5319-5331.
16. H.-X. Zhou, A. Szabo, J. F. Douglas, and J. B. Hubbard (1994), *A Brownian dynamics algorithm for calculating the hydrodynamic friction and the electrostatic capacitance of an arbitrarily-shaped object*. J. Chem. Phys. **100**, 3821-3826.
15. H.-X. Zhou (1994), *Macromolecular electrostatic energy within the nonlinear Poisson-Boltzmann equation*. J. Chem. Phys. **100**, 3152-3162.
14. O. Schaad, H.-X. Zhou, A. Szabo, W. A. Eaton, and E. R. Henry (1993), *Simulation of the kinetics of ligand binding to a protein by molecular dynamics: geminate rebinding of nitric oxide to myoglobin*. Proc. Natl. Acad. Sci. USA **90**, 9547-9551.
13. H.-X. Zhou (1993), *Boundary element solution of macromolecular electrostatics: interaction energy between two proteins*. Biophys. J. **65**, 955-963.
12. H.-X. Zhou (1993), *Brownian dynamics study of the influences of electrostatic interaction and diffusion on protein-protein association kinetics*. Biophys. J. **64**, 1711-1726.
11. H.-X. Zhou (1993), *Dynamic spherical model for solvation in a dipolar lattice*. J. Phys. Chem. **97**, 4216-4223.
10. H.-X. Zhou, B. Bagchi, A. Papazyan, and M. Maroncelli (1992), *Solvation dynamics in a Brownian dipole lattice: a comparison between theory and computer simulation*. J. Chem. Phys. **97**, 9311-9320.
9. B. A. Luty, J. A. McCammon, and H.-X. Zhou (1992), *Diffusive reaction rates from Brownian dynamics simulations: replacing the outer cut-off surface by an analytical treatment*. J. Chem. Phys. **97**, 5682-5686.
8. H.-X. Zhou and B. Bagchi (1992), *Dielectric and orientational relaxation in a Brownian dipolar lattice*. J. Chem. Phys. **97**, 3610-3620.
7. H.-X. Zhou and A. Szabo (1991), *Comparison between molecular dynamics simulations and the Smoluchowski theory of reactions in a hard sphere liquid*. J. Chem. Phys. **95**, 5948-5952.
6. H.-X. Zhou and R. Zwanzig (1991), *A rate process with an entropy barrier*. J. Chem. Phys. **94**, 6147-6152.
5. H.-X. Zhou (1990), *Kinetics of diffusion-influenced reactions studied by Brownian dynamics*. J. Phys. Chem. **94**, 8794-8800.
4. H.-X. Zhou and F. A. Ferrone (1990), *Theoretical description of the spatial dependence of sickle hemoglobin polymerization*. Biophys. J. **58**, 695-703.
3. H.-X. Zhou and A. Szabo (1990), *Mean field theory of transient fluorescence quenching in the frequency domain*. J. Chem. Phys. **92**, 3874-3880.
2. H.-X. Zhou (1990), *On the calculation of diffusive reaction rates using Brownian dynamics simulations*. J. Chem. Phys. **92**, 3092-3095.
1. H.-X. Zhou (1989), *The exponential nature of barrier crossings studied by Langevin dynamics*. Chem. Phys. Lett. **164**, 285-290.

Invited Talks (since 2007)

2019 (partial)

Workshop on “Mathematics Biophysics and Molecular Biosciences”, Tsinghua Sanya International Mathematics Forum
 International Symposium of Phase Separation and Phase Transition in Biological Systems, Hefei, China
 Department of Chemistry, University of Arkansas
 Department of Chemistry, University of Albany
 Center for Computational Biology, University of Kansas
 Center for Quantitative Biology, Peking University, China
 NYU-ECNU Center for Computational Chemistry, New York University Shanghai

Department of Chemistry, Fudan University, China
Fifth Symposium on “Biophysics Postgraduate Research in Hong Kong”, Chinese University of Hong Kong
Telluride Workshop on “Ion Channel Biophysics”, Colorado
Telluride Workshop on “Macromolecular Crowding”, Colorado
Laufer Center for Physical and Quantitative Biology, Stony Brook University
Laboratory of Chemical Physics, National Institutes of Health
NSF-CBMS Conference: Mathematical Molecular Bioscience and Biophysics, University of Alabama
American Chemical Society Spring National Meeting, Orlando
Greater Boston Area Theoretical Chemistry Lecture, MIT/Harvard/Boston University
American Physical Society March National Meeting, Boston

2018

Theoretical and Computational Biophysics Group, University of Illinois at Urbana-Champaign
Conference on “Modeling of Protein Interactions”, University of Kansas
GDCh colloquium, Technische Universität Braunschweig, Germany
Department of Physiology and Biophysics, Rush University
Department of Chemistry, Illinois Institute of Technology
Conference on Pulse Investigations in Chemistry, Physics, and Biology, Lodz, Poland
Institute for Advanced Simulations, Forschungszentrum Jülich, Germany
Workshop on “Biological Diffusion and Brownian Dynamics Brainstorm 4”, Heidelberg, Germany
Department of Physics, Technical University of Munich, Germany
Center for Bioinformatics, Saarland University, Germany
Department of Chemistry, University of Oxford, UK
Department of Biology, Chemistry, and Pharmacy, Free University of Berlin, Germany
Department of Biochemistry, University of Zurich, Switzerland
Max Planck Institute of Biophysics, Frankfurt, Germany
HGS MathComp Romberg Inaugural Lecture, Heidelberg University

2017

Department of Biomolecular Science, Weizmann Institute of Science
Department of Microbiology and Molecular Genetics, Hebrew University
Conference on “Molecular Perspectives on Protein-Protein Interactions”, Eilat, Israel
Department of Physics, Wuhan University, China
Wang TC Lecture, Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences
Bioinformatics Institute, Singapore
School of Biological Sciences, Nanyang Technological University, Singapore
Singapore-MIT Alliance for Research and Technology (SMART), Singapore
School of Physics, Huazhong University of Science and Technology, China
Department of Chemistry, Kyoto University
Department of Physics, Nagoya University
Theoretical Molecular Science Laboratory, RIKEN, Japan
Annual Meeting of the Biophysical Society of Japan, Kumamoto
Department of Biomedical and Pharmaceutical Sciences, University of Montana
American Chemical Society Fall National Meeting, Washington DC
Telluride Workshop on “Ion Channel Biophysics”, Colorado
Telluride Workshop on “Protein Electrostatics”, Colorado
Telluride Workshop on “Macromolecular Crowding”, Colorado
Florida Section of the American Chemical Society Annual Meeting
Department of Physics, University of Illinois Chicago
American Chemical Society Spring National Meeting, San Francisco
American Physical Society March National Meeting, New Orleans

Department of Chemistry, University of Illinois Chicago
Department of Chemistry, University of Colorado Denver
Department of Biochemistry and Structural Biology, University of Texas Health Science Center at San Antonio

2016

Workshop on “Mathematics Biophysics and Molecular Biosciences”, Tsinghua Sanya International Mathematics Forum
“Science at the Edge” Seminar, Michigan State University
Conference on “Modeling of Protein Interactions”, University of Kansas
Department of Physics, University of Houston
American Chemical Society Fall National Meeting, Philadelphia
Workshop on “Frontiers in Molecular Biophysics”, NYU-ECNU Center for Computational Chemistry, New York University Shanghai
NYU-ECNU Center for Computational Chemistry, New York University Shanghai
Department of Physics, Fudan University
School of Chemistry and Chemical Engineering, Nanjing University
Kuang Yaming Honors School, Nanjing University
Telluride Workshop on “Protein and Peptide Interactions in Cellular Environments”, Colorado
Focused Program on “Molecular Machines of Life: Simulation Meets Experiment”, Institute for Advanced Study, Hong Kong University of Science and Technology
Department of Physics, Chinese University of Hong Kong
Center for Computational Biology and Bioinformatics, Indiana University School of Medicine
Sixth CAPRI Evaluation Meeting, Tel Aviv, Israel
Department of Chemistry, University of South Florida
American Chemical Society Spring National Meeting, San Diego

2015

Biophysics Graduate Program, Ohio State University
Workshop on “Modeling and Computation of Transmembrane Transport”, Ohio State University
Department of Physics, Arizona State University
Workshop on “Multiple Faces of Biomolecular Electrostatics”, Ohio State University
American Chemical Society Fall National Meeting, Boston
Telluride Workshop on “Ion Channel Biophysics”, Colorado
Snowmass Workshop on “Free Energy Calculations”, Colorado
Albany 2015: 19th Conversation, State University of New York at Albany
Department of Biochemistry & Molecular Biophysics, Kansas State University
Department of Physics, University of Missouri-Columbia
American Chemical Society Spring National Meeting, Denver
Laboratory of Computational Biology, NIHBL, National Institutes of Health

2014

Conference on “Modeling of Protein Interactions”, University of Kansas
Department of Chemical and Biomedical Engineering, FAMU-FSU College of Engineering
Telluride Workshop on “Molecular Recognition”
Conference on “Reaction Kinetics in Soft and Condensed Matter”, Orléans, France
Department of Physics and Astronomy, Clemson University
Department of Physics, University of Missouri-Columbia
Life Sciences Symposium, College of Medicine, Florida State University
Department of Cell Biology, Microbiology and Molecular Biology, University of South Florida

2013

Workshop on “Computer Modeling of Complex Processes”, Hong Kong University
Department of Chemistry, Hong Kong University of Science and Technology

Workshop on “Biological Diffusion and Brownian Dynamics Brainstorm 3”, Heidelberg, Germany
Department of Computational Medicine and Bioinformatics, University of Michigan
Department of Chemistry and Chemical Biology, Indiana University-Purdue University Indianapolis
American Chemical Society Fall National Meeting, Indianapolis
27th Symposium of the Protein Society, Boston
Snowmass Summer Biophysics Workshop on “Free Energy Calculations”, Colorado
Department of Chemistry, Seoul National University
StatPhys 25 Satellite Meeting “Stochastic Transport and Reaction Processes in Condensed Media”, Jeju
Island, Korea
National Institute of Biological Sciences, Beijing
Institute of High Energy Physics, Chinese Academy of Sciences, Beijing
Institute of Physics, Chinese Academy of Sciences, Beijing
Program on “Small System Nonequilibrium Fluctuations, Dynamics and Stochastics, and Anomalous
Behavior”, Kavli Institute for Theoretical Physics China, Beijing
College of Chemistry and Chemical Engineering, Lanzhou University, China
Center for Quantitative Biology, Peking University, Beijing
Program on “Advanced Molecular Simulation Methods in the Physical Sciences”, Kavli Institute for
Theoretical Physics China, Beijing
School of Physics, Huazhong University of Science and Technology, China
School of Life Sciences, University of Science and Technology of China, Hefei
School of Medicine, Soochow University, China
Fifth CAPRI Evaluation Meeting, Utrecht, The Netherlands
Distinguished Lecture in Mathematical and Computational Biology, University of California at Irvine

2012

Department of Chemistry, Georgia State University
Conference on “Modeling of Protein Interactions”, University of Kansas
CMU-Pitt PhD Program in Computational Biology
American Chemical Society Fall National Meeting, Philadelphia
Department of Biochemistry, University of Zurich, Switzerland
Centro Stefano Franscini Conference on “Molecular Crowding: Chemistry and Physics Meet Biology”,
Monte Verità, Switzerland
American Chemical Society Spring National Meeting, San Diego
Department of Chemistry, Rice University
Department of Chemistry and Biochemistry, University of California at Santa Barbara
Biophysical Society Biopolymers in Vivo Subgroup Symposium, San Diego
Department of Chemistry and Biochemistry, University of California at San Diego

2011

Department of Chemistry, Seoul National University
School of Computational Sciences, Korea Institute for Advanced Study
Department of Biomedical Engineering, Pukyong National University, Korea
Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences
School of Physics, Huazhong University of Science and Technology, China
Department of Physics, Wuhan University, China
School of Physics, Georgia Institute of Technology
Department of Physics, University of Illinois at Chicago
American Chemical Society Fall National Meeting, Denver
Telluride Workshop on “Ion Channel Biophysics”
CECAM Workshop on “Dynamics and Thermodynamics of Biomolecular Recognition”, Ecole
Polytechnique, Palaiseau, France
Conference on “Modeling Electrostatics in Molecular Biology”, Clemson University

American Physical Society March National Meeting, Dallas

2010

Institute of Computational Engineering and Sciences, University of Texas Austin
 Conference on “Modeling of Protein Interactions”, University of Kansas
 Southeastern Magnetic Resonance Conference, Gainesville, Florida
 Workshop on “Biological Diffusion and Brownian Dynamics Brainstorm 2”, Heidelberg, Germany
 24th Annual Gibbs Conference on Biothermodynamics, Carbondale, Illinois
 Conference on “Reaction Kinetics in Condensed Matter”, Moscow, Russia
 Telluride Workshop on “Protein and Peptide Interactions in Cellular Environments”, Colorado
 School of Physics, Huazhong University of Science and Technology, China
 Department of Mathematics, University of South Carolina
 Biophysical Society IDP Subgroup Symposium, San Francisco

2009

Fourth CAPRI Evaluation Meeting, Barcelona, Spain
 CECAM Workshop on “Linking Systems Biology and Biomolecular Simulations”, Lausanne, Switzerland
 Program on “Function and Dynamics of Biomolecules”, Kavli Institute for Theoretical Physics China, Beijing
 Institute of Computational Mathematics and Scientific/Engineering Computing, Chinese Academy of Sciences, Beijing
 College of Life Sciences, Wuhan University, China
 Department of Physics, University of Denver
 Department of Chemistry, Stanford University
 Beckman Research Institute, City of Hope
 Department of Mathematics, University of California at San Diego
 Center for Theoretical Biological Physics, University of California at San Diego
 Department of Biochemistry and Molecular Biophysics, Columbia University
 Department of Chemistry, New York University
 Institute of Biophysics, Chinese Academy of Sciences, Beijing
 Department of Chemistry and Biochemistry, University of California at Santa Cruz

2008

Greater Boston Area Theoretical Chemistry Lecture, MIT
 Department of Physics, Brandeis University
 INRIA Sophia-Antipolis, France
 IBBMC Université de Paris-Sud 11, France
 ISIS Université Louis Pasteur, France
 American Chemical Society Fall National Meeting, Philadelphia
 Department of Physics, Duke University
 Telluride Workshop on “Protein Electrostatics”, Colorado
 Telluride Workshop on “Enhanced Sampling”, Colorado
 Conference on “Molecular Perspectives on Protein-Protein Interactions”, Croatia
 Gordon Conference on Biopolymers, Salve Regina University, Rhode Island
 Department of Chemistry, University of Pennsylvania

2007

College of Life Sciences, Wuhan University, China
 Conference on “Modeling of Protein Interactions”, University of Kansas
 American Chemical Society Fall National Meeting, Boston
 Laboratory of Chemical Physics, NIDDK, National Institutes of Health
 Department of Physics, Drexel University
 Third CAPRI Evaluation Meeting, Toronto

Department of Biochemistry, University of Toronto
American Chemical Society Spring National Meeting, Chicago
Department of Physics, University of Illinois at Chicago
Department of Chemistry, Duke University
University of Maryland Biotechnology Institute