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 BBCA 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-, 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) Allostery and binding kinetics of structured and disordered proteins; (2) Crowding and emergent properties in cellular environments; (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 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 AG045703, *Solid State NMR Structural Analysis of Oligomeric Alzheimer's Beta-Amyloid Peptide* (2014-2019) (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

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. (in press).
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 RIα 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. Kryshtafovych, 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. Borrman, 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. Kastritis, 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. Férnandez-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. Fernendez-Recio, J. Xu, P. Muthu, K. P. Kilambi, J. J. Gray, S. Grudinin, 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. Rooman, 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. Grudinin, J. Esquivel-Rodríguez, 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). *PI^{2}PE: 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 H_2O/D_2O 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.
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Invited Talks (since 2007)

2018 (partial)

Conference on "Modeling of Protein Interactions", University of Kansas
GDCh colloquium, Technische Universität Braunschweig, Germany
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