

# 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

## Positions

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

2020-, Scientific Advisory Board, Adagene Inc.

## Honors

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

2011, Distinguished Research Professor, Florida State University

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)

2022-2023, Chair, Biopolymers in Vivo Subgroup, Biophysical Society

2020, Secretary-Treasurer, Division of Biological Physics, American Physical Society

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

2010, Co-Chair, IDP Subgroup Symposium, Biophysical Society

2018 & 2022, DFG Review Panel

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

2021 & 2022, NSF Review Panel

2022-, Faculty Reviews: Landmark Advisory Board

2021-, Associate Editor, Frontiers in Molecular Biosciences

2020-2022, Co-Editor, Methods in Molecular Biology volume on Phase-Separated Biomolecular Condensates

2014-2018, Editorial Board, Protein Engineering, Design and Selection

2016-2019, Biophysics Subject Editor, Elsevier's Life Science Reference Module

2008-2018, 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

2009 & 2011, Organizer, Telluride Workshop on Macromolecular Crowding

2009, Organizer, ACS Symposium on Protein Dynamics and Function,

2020-, Scientific Advisory Board, Adagene Inc.

## Research Interests

Combining theory, computation, and experiment to address a range of topics in molecular and cellular biophysics. Four main areas are: (1) thermodynamic and dynamic properties of phase-separated biomolecular condensates; (2) membrane association and binding kinetics of intrinsically disordered proteins; (3) structures and pathways of the self-assemblies of amyloid- $\beta$  and other amyloidogenic proteins; and (4) functional mechanisms of glutamate-receptor ion channels.

### Current Grants

Principal Investigator, NIH Grant R35 GM118091, *Quantitative, Mechanistic Studies of Biomolecular Recognition* (2016-2026).

Principal Investigator, NIH Grant R35 GM118091-07S1, *Administrative Supplement to Acquire a GPU Cluster* (2022-2026).

Multiple Principal Investigator, NIH Grant RF1 AG073434, *Characterizing Alzheimer's Amyloid-beta Oligomer Structures by Solid-State NMR and Cryo-Electron Microscopy* (2022-2025).

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

### 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

- 291.G. Hu and H.-X. Zhou (2023). *Magnesium ions mediate ligand binding and conformational transition of the SAM/SAH riboswitch*. BioRxiv.
- 290.S. Qin and H.-X. Zhou (2023). *Predicting the sequence-dependent backbone dynamics of intrinsically disordered proteins*. bioRxiv.
- 289.S. Dey and H.-X. Zhou (2023). *Why does synergistic activation of WASP, but not N-WASP, by Cdc42 and PIP2 require Cdc42 prenylation?* J. Mol. Biol. **435**, 168035.
- 288.J. Amin, M. He, R. Prasad, X. Leng, H.-X. Zhou, and L.P. Wollmuth (2023). *Two gates mediate NMDA receptor activity and are under subunit-specific regulation*. Nat. Commun. (in press).
- 287.S. T Smrt, C. A. Escobar, S. Dey, T. A. Cross, and H.-X. Zhou (2023). *An Arg/Ala-rich helix in the N-terminal region of M. tuberculosis FtsQ anchors FtsZ to membranes*. Commun. Biol. (in press).
- 286.S. Dey and H.-X. Zhou (2023). *N-WASP is competent for downstream signaling before full release from autoinhibition*. J. Chem. Phys. **158**, 091105.
- 285.M. MacAinsh and H.-X. Zhou (2023). *Partial mimicry of the microtubule binding of tau by its membrane binding*. Protein Sci. **32**, e4581.
- 284.A. Ghosh, D. Kota, and H.-X. Zhou (2023). *Determining thermodynamic and material properties of biomolecular condensates by confocal microscopy and optical tweezers*. Methods Mol. Biol. **2563**, 237-260.
- 283.K. Mazarakos, S. Qin, and H.-X. Zhou (2023). *Calculating binodals and interfacial tension of phase-separated condensates from molecular simulations with finite-size corrections*. Methods Mol. Biol. **2563**, 1-35.
- 282.D. A. Agard, G. R. Bowman, W. DeGrado, N. V. Dokholyan, and H.-X. Zhou (2022). *Solution of the protein structure prediction problem at last: crucial innovations and next frontiers*. Faculty Rev. **11**, 38.
- 281.T. L. Rosenberry, H. X. Zhou, S. M. Stagg, and A. K. Paravastu (2022). *Oligomer formation by amyloid- $\beta$ 42 in a membrane-mimicking environment in Alzheimer's disease*. Molecules **27**, 8804.
- 280.K. Mazarakos, R. Prasad, and H.-X. Zhou (2022). *SpiDec: Computing binodals and interfacial tension of biomolecular condensates from simulations of spinodal decomposition*. Front. Mol. Biosci. **9**, 1021939.
- 279.S. Dey, M. MacAinsh, and H.-X. Zhou (2022). *Membrane tethering of SepF, a membrane anchor for the mycobacterium tuberculosis Z-ring*. J. Mol. Biol. **434**, 167817.

- 278.S. Dey, M. MacAinsh, and H.-X. Zhou (2022). *Sequence-dependent backbone dynamics of intrinsically disordered proteins*. J. Chem. Theory Comput. **18**, 6310-6323.
- 277.S. Qin, A. Hicks, S. Dey, R. Prasad, H.-X. Zhou (2022). *ReSMAP: Web server for predicting residue-specific membrane-association propensities of intrinsically disordered proteins*. Membranes **12**, 773.
- 276.D. Kota and H.-X. Zhou (2022). *Macromolecular regulation of the material properties of biomolecular condensates*. J. Phys. Chem. Lett. **13**, 5285-5290.
- 275.A. Gupta, S. Dey, and H.-X. Zhou (2022). *Artificial intelligence guided conformational mining of intrinsically disordered proteins*. Commun. Biol. **5**, 610.
- 274.K. Mazarakos and H.-X. Zhou (2022). *Multiphase organization is a second phase transition within multi-component biomolecular condensates*. J. Chem. Phys. **156**, 191104.
- 273.X. Dong, L.-Y. Qin, Z. Gong, S. Qin, H.-X. Zhou, and C. Tang (2022). *Preferential interactions of a crowder protein with the specific binding site of a native protein complex*. J. Phys. Chem. Lett. **13**, 792-800.
- 272.G. Hu and H.-X. Zhou (2021). *Binding free energy decomposition and multiple unbinding paths of buried ligands in a PreQ<sub>1</sub> riboswitch*. PLoS Comput. Biol. **17**, e1009603.
- 271.A. Ghosh, D. Kota, and H.-X. Zhou (2021). *Shear relaxation governs fusion dynamics of biomolecular condensates*. Nat. Commun. **12**, 5995.
- 270.H.-X. Zhou (2021). *Shape recovery of deformed biomolecular droplets: Dependence on condensate viscoelasticity*. J. Chem. Phys. **155**, 145102.
- 269.A. Hicks, M. MacAinsh, and H.-X. Zhou (2021). *Removing thermostat distortions of protein dynamics in constant-temperature molecular dynamics simulations*. J. Chem. Theory Comput. **17**, 5920-5932.
- 268.A. Gupta and H.-X. Zhou (2021). *Machine learning-enabled pipeline for large-scale virtual drug screening*. J. Chem. Inf. Model. **61**, 4236-4244.
- 267.S.-H. Ahn, S. Qin, J. Z. Zhang, J. A. McCammon, J. Zhang, and H.-X. Zhou (2021). *Characterizing protein kinase A (PKA) subunits as macromolecular regulators of PKA RI $\alpha$  liquid-liquid phase separation*. J. Chem. Phys. **154**, 221101.
- 266.Y. Yang, H. Dong, and H.-X. Zhou (2021). *Effects of cholesterol on the partitioning of a drug molecule in lipid bilayers*. J. Phys. Chem. B **125**, 5338-5345.
- 265.K. Mazarakos and H.-X. Zhou (2021). *Macromolecular regulators have matching effects on the phase equilibrium and interfacial tension of biomolecular condensates*. Protein Sci. **30**, 1360-1370.
- 264.H.-X. Zhou (2021). *Viscoelasticity of biomolecular condensates conforms to the Jeffreys model*. J. Chem. Phys. **154**, 041103.
- 263.A. Hicks, C. A. Escobar, T. A. Cross, and H.-X. Zhou (2021). *Fuzzy association of an intrinsically disordered protein with acidic membranes*. JACS Au **1**, 66-78.
- 262.A. Gupta and H.-X. Zhou (2020). *Profiling SARS-CoV-2 main protease (M<sup>PRO</sup>) binding to repurposed drugs using molecular dynamics simulations in classical and neural network-trained force fields*. ACS Comb. Sci. **22**, 826-832.
- 261.H.-X. Zhou (2020). *Determination of condensate material properties from droplet deformation*. J. Phys. Chem. B **124**, 8372-8379.
- 260.A. Ghosh and H.-X. Zhou (2020). *Determinants for fusion speed of biomolecular droplets*. Angew. Chem. Int. Ed. **59**, 20837-20840.
- 259.A. Hicks, C. A. Escobar, T. A. Cross, and H.-X. Zhou (2020). *Sequence-dependent correlated segments in the intrinsically disordered region of ChiZ*. Biomolecules **10**, 946.
- 258.R. Prasad and H.-X. Zhou (2020). *Membrane association and functional mechanism of synaptotagmin-1 in triggering vesicle fusion*. Biophys. J. **119**, 1255-1265.
- 257.Y. Gao, C. Guo, J. O. Watzlawik, E. J. Lee, D. Huang, H.-X. Zhou, T. L. Rosenberry, and A. Paravastu (2020). *Out-of-register parallel  $\beta$ -sheets and antiparallel  $\beta$ -sheets coexist in 150 kDa oligomers formed by Amyloid- $\beta$ (1-42)*. J. Mol. Bio. **432**, 4388-4407.
- 256.A. Ghosh, X. Zhang, and H.-X. Zhou (2020). *Tug of war between condensate phases in a minimal macromolecular system*. J. Am. Chem. Soc. **142**, 8848-8861.

255. J. Paulino, M. Yi, I. Hung, Z. Gan, X. Wang, E. Y. Chekmenev, H.-X. Zhou, and T. A. Cross (2020). *Functional stability of water wire-carbonyl interactions in an ion channel*. Proc. Natl. Acad. Sci. USA **117**, 11908–11915.
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  $\text{A}\beta$  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  $\text{Ca}^{2+}$  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 R1 $\alpha$  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  $\beta$ -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  $\alpha$ -amino-3-hydroxy-5-methyl-4-isoxazolepropionic acid (AMPA) receptors*. *J. Biol. Chem.* **291**, 6595-6606.
- 220.M. F. Lensink, S. Velankar, A. Kryshchuk, 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. Maignet, 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. Joungh, 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  $\alpha$* . *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.
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8. H.-X. Zhou and B. Bagchi (1992), *Dielectric and orientational relaxation in a Brownian dipolar lattice*. J. Chem. Phys. **97**, 3610-3620.
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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.
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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)

2023 (partial)

American Chemical Society Spring National Meeting, Indianapolis  
 Conference on “Modeling of Protein Interactions”, University of Kansas  
 Telluride Workshop on “Macromolecular Crowding”, Colorado  
 CECAM Workshop “Making the invisible protein life visible using integrative biophysical approaches”,  
 Lugano, Switzerland

2022

US LUMICKS C-Trap User Meeting, Rockefeller University  
 Department of Physics, Indiana University-Purdue University Indianapolis  
 Conference on “Topology-based Learning, Biomolecular Topology and Related Topics”, Institute for  
 Mathematical Sciences, Singapore  
 Center for Life Sciences, Peking University and Tsinghua University, China  
 American Chemical Society Spring National Meeting, San Diego  
 CECAM Workshop “From disordered biomolecular complexes to biological coacervates”, Zurich,  
 Switzerland  
 American Physical Society March Meeting, Chicago

2021

Workshop on “Computational and Mathematical Bioinformatics and Biophysics”, Tsinghua Sanya  
 International Mathematics Forum  
 Research Day Keynote Lecture, Center for Bioinformatics and Quantitative Biology, University of  
 Illinois at Chicago  
 Department of Physics, University at Buffalo, SUNY  
 Department of Chemistry and Chemical Biology, Rutgers University

Meeting on Advancing the Physicochemical Principles of Protein-Protein Interactions, Laufer Center for Physical and Quantitative Biology, Stony Brook University  
American Chemical Society Fall National Meeting  
Workshop on “Mathematics in Action: Modeling and Analysis in Molecular Biology and Electrophysiology”, Duke Kunshan University  
American Chemical Society Spring National Meeting  
Protein Electrostatics Conference, Hosted by Istituto Italiano di Tecnologia

2020

Workshop on “Computational and Mathematical Bioinformatics and Biophysics”, Tsinghua Sanya International Mathematics Forum  
Workshop for Protein Complexes and Quantitative Proteomics, Renmin University of China  
The Third Worldwide Chinese Computational Biology Conference, Peking University

2019

School of Pharmaceutical Sciences, Sun Yat-Sen University, China  
Shenzhen Bay Laboratory  
Department of Chemistry, Southern University of Science and Technology of China  
School of Life and Health Sciences, Chinese University of Hong Kong Shenzhen  
School of Chemical Biology and Biotechnology, Peking University Shenzhen  
Workshop on “Computational and Mathematical Bioinformatics and Biophysics”, 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