Yinghao Wu, Ph.D.

Department of Systems and Computational Biology
Michael F. Price Center for Genetic and Translational Medicine
Albert Einstein College of Medicine
1301 Morris Park Avenue, Rm 553A
Bronx, NY 10461
Phone: 718-678-1232 (Office) and 718-678-1018 (Fax)
Email: yinghao.wu@einstein.yu.edu
Web: http://www.columbia.edu/ ~yw2286

Scientific Employment

06/2018 – Present	Associate Professor, Department of Systems and Computational Biology Albert Einstein College of Medicine
10/2012 – 06/2018	Assistant Professor, Department of Systems and Computational Biology Albert Einstein College of Medicine
01/2008 – 10/2012	Postdoctoral Research Scientist, Howard Hughes Medical Institute, Center for Computational Biology and Bioinformatics, Dept. of Biochemistry and Molecular Biophysics, Columbia University, New York, NY, USA

Education

01/2008	Ph.D. in Applied Physics and Bioengineering, Applied Physics Program/Dept. of Bioengineering, Rice University, Houston, TX, USA
06/2002	M.S. in Physics, Dept. of Physics/Fudan Surface Physics National Key Laboratory Fudan University, Shanghai, China
06/1999	B.S. in Physics, Dept. of Physics, Fudan University, Shanghai, China

Selected Awards & Honors

2011	Semifinalist, Earl Stadtman Investigator, National Institute of Health
2011	CBSB Outstanding Young Researcher Award, Julich Research Center, Germany
2010	Outstanding Poster Award for 13th NY Structural Biology Discussion Group
2006	Best Presentation of 20th Rice Quantum Institute Annual Research Colloquium
2002 – 2003	Dean's Fellowship, Rice University
1998 – 1999	First Grade of People's Scholarship of Fudan University
1997 – 1998	Excellent Student Scholarship (Laureate ship) of Fudan University

Funding Support

Current:

1. 1R01GM120238 (Yinghao, PI) 9/1/2016-7/31/2021 6.0 calendar months
   NIH/NIGMS $197,500.00
   A multiscale model for binding kinetics of membrane receptors on cell surfaces
2. 1R01GM122804 (Yinghao, PI) 9/1/2017-7/31/2021 5.0 calendar months
   NIH/NIGMS $196,250.00
   Computational models for the signaling of tumor necrosis factor receptor on cell surfaces
3. 1R01GM117104 (Yinghao, co-I) 9/30/2017-7/31/2021 1.0 calendar months
   NIH/NIGMS $22,947.00
   Multiscale Investigation of the Impact of 2D Confinement on Adhesion Protein Function

Publications

1. J. Chen and **Y. Wu***, "A multi-scale computational model for simulating the kinetics of protein complex assembly ". ***Methods in Molecular Biology: Protein Complex Assembly*** (**2018**) 1764: 401-411.
2. J. Chen, B. Wang and **Y. Wu***, "Structural Characterization and Function Prediction of Immunoglobulin-like Fold in Cell Adhesion and Cell Signaling". ***Journal of Chemical Information and Modeling*** (**2018**) 58(2):532-542.
3. J. Chen, S. Almo and **Y. Wu***, " General principles of binding between cell surface receptors and multi-specific ligands: A computational study ". ***PLOS Computational Biology*** (**2017**) 13(10):e1005805.
4. Z. Xie, J. Chen and **Y. Wu***, "Predicting Protein-protein Association Rates using Coarse-grained Simulation and Machine Learning". ***Scientific Reports*** (**2017**) 7: 46622.
5. J. Chen and **Y. Wu***, "Understanding the Functional Roles of Multiple Extracellular Domains in Cell Adhesion Molecules with a Coarse-Grained Model". ***Journal of Molecular Biology*** (**2017**) 429: 1081-1095.
6. J. Chen, Z. Xie and **Y. Wu***, "Understand protein functions by comparing the similarity of local structural environments". ***Biochimica et Biophysica Acta: Proteins and Proteomics*** (**2017**) 1865: 142-152.
7. J. Chen, J Newhall, Z Xie, D Leckband and **Y Wu***, “A Computational Model for Kinetic Studies of Cadherin Binding and Clustering”. ***Biophysical Journal*** (**2016**) 111: 1507-1528.
8. J. Chen, Z. Xie and **Y. Wu***, "Elucidating the Functional Roles of Spatial Organization in Cross-Membrane Signal Transduction by a Hybrid Simulation Method". ***Journal of Computational Biology*** (**2016**) Mar 30. PMID: 27028148
9. Z. Xie, J. Chen and **Y. Wu***, "Multiscale Model for the Assembly Kinetics of Protein Complexes". ***J. Physical Chemistry B*** (**2016**) 120(4):621-32. doi: 10.1021/acs.jpcb.5b08962.

10. J. Chen, Z. Xie and **Y. Wu***, "Elucidating the general principles of cell adhesion with a coarse-grained simulation model". ***Molecular BioSystems*** (**2016**) 12(1):205-18. doi: 10.1039/c5mb00612k.

11. J. Chen, Z. Xie and **Y. Wu***, "Study of protein structural deformations under external mechanical perturbations by a coarse-grained simulation method". ***Biomechanics and Modeling in Mechanobiology*** (**2016**) 12(1):205-18. doi: 10.1039/c5mb00612k.

12. Z. Xie, J. Chen, Y. Zhao and **Y. Wu***, "Decomposing the space of protein quaternary structures with the interface fragment pair library". ***BMC Bioinformatics*** (**2015**) 16: 14. doi:10.1186/s12859-014-0437-4

13. Z. Xie, J. Chen and **Y. Wu***, "Linking 3D and 2D binding kinetics of membrane proteins by multi-scale simulations". ***Protein Science*** (**2014**) doi: 10.1002/pro.2574.

14. J. Chen, Z. Xie and **Y. Wu***, "Computational Modeling of the Interplay between Cadherin-Mediated Cell Adhesion and Wnt Signaling Pathway". ***PLoS ONE*** (**2014**) 9(6): e100702. doi:10.1371/journal.pone.0100702.

15. J. Chen, Z. Xie and **Y. Wu***, "A multiscale model for simulating binding kinetics of proteins with flexible linkers". ***Proteins: Structure, Function, and Bioinformatics*** (**2014**) Oct; 82(10):2512-22.

16. Z. Xie, J. Chen and **Y. Wu***, "A coarse-grained model for the simulations of biomolecular interactions in cellular environments". ***Journal of Chemical Physics*** (**2014**) 140: 054112.

17. **Y. Wu**, B. Honig and A. Ben-Shaul, "Theory and Simulations of Adhesion Receptor Dimerization on Membrane Surfaces". ***Biophysical Journal*** (**2013**) 104: 1221-1229.

18. **Y. Wu**, J. Vendome, L. Shapiro, A. Ben-Shaul and B. Honig, "Transforming binding affinities from 3D to 2D with application to cadherin clustering". ***Nature*** (**2011**) 475, 510-513.

19. O. Harrison, X. Jin, S. Hong, F. Bahna1, G. Ahlsen, J. Brasch, **Y. Wu**, J. Vendome, K. Felsovalyi, etc. "The extracellular architecture of adherens junctions revealed by crystal structures of type I cadherins". ***Structure*** (**2011**) 19, 244-256**.**

20. **Y. Wu**, X. Jin, O. Harrison, L. Shapiro, B. Honig and A. Ben-Shaul, "Cooperativity between trans and cis interactions in cadherin-mediated junction formation". ***P.N.A.S.*** (**2010**) 107 (41) 17592-17597.

21. **Y. Wu**, AD. Dousis, M. Chen, J. Li, and J. Ma, "OPUS-Dom: Applying the Folding-Based Method VECFOLD to Determine Protein Domain Boundaries". ***J. Mol. Biol.*** (**2009**) 385, 1314-1329.

22. M. Chen, AD. Dousis, **Y. Wu**, and J. Ma, "Predicting protein folding cores by empirical potential functions". ***Archives of Biochemistry and Biophysics*** (**2009**) 483, 16-22.

23. **Y. Wu**, M. Lu, M. Chen, J. Li, and J. Ma, "OPUS-Ca: A knowledge-based potential function requiring only C-α Positions". ***Protein Science*** (**2007**) 16, 1449-1463.

24. M. Chen, C.J. Wilson, **Y. Wu**, P. Wittung-Stafshede, and J. Ma, "Correlation between Protein Stability Cores and Protein Folding Kinetics: A Case Study on Pseudomonas aeruginosa Apo-Azurin". ***Structure*** (**2006**) 14, 1-10.

25. **Y. Wu**, X. Tian, M. Lu, M. Chen, Q. Wang and J. Ma, "Folding of Small Helical Proteins Assisted by Small-Angle X-Ray Scattering Profiles". ***Structure*** (**2005**) 13, 1587-1597.

26. Y. Yuan, **Y. Wu** and J. Zi, "Heat Capacities of Globular Proteins". ***J. of Phys.: Condensed Matter,*** (**2005**) 17, 469-473.

27. **Y. Wu**, M. Chen, M. Lu, Q. Wang and J. Ma, "Determining Protein Topology from Skeletons of Secondary Structures". ***J. Mol. Biol.*** (**2005**) 350, 571-586.
28. **Y. Wu** and J. Ma, "Normal-mode-based Refinement of an F-actin Model Against Fiber Diffraction Data". ***Fiber Diffraction Review,*** (2004) 12, 25-28.
29. **Y. Wu** and J. Ma, "Refinement of F-actin Model against Fiber Diffraction Data by Long-Range Normal Modes". ***Biophysical J.*** (**2004**) 86, 116-124.
30. D. Ming, Y. Kong, **Y. Wu** and J. Ma, "Simulation of F-actin filaments of Several Microns". ***Biophysical J.*** (**2003**) 85, 27-35.
31. Y. Kong, D. Ming, **Y. Wu**, J. Stoops, H. Zhou and J. Ma, "Conformational Flexibility of Pyruvate Dehydrogenase Complexes: A Computational Analysis by QEDM". ***J. Mol. Biol.*** (**2003**) 330, 129-135.
32. D. Ming, Y. Kong, **Y Wu** and J. Ma, "Substructure Synthesis Method for Simulating Large Molecular Complexes". ***P.N.A.S***. (**2003**) 100, 104-109.
33. **Y. Wu** and J. Zi, "Universal Behavior of Localization of Residue Fluctuations in Globular Proteins". ***Physical Reviews E***. (**2003**) 67, 041909-041912.

Invited Talks

1. "Multi-scale Modeling of Protein-protein Interactions for Understanding the Molecular Mechanisms of Cell adhesion and Signaling". New York Structural Biology Discussion Group Winter Meeting, New York, NY, January, 2018
2. "Understand Binding Kinetics of Membrane Receptors and Their Functional Roles in Cell adhesion and Signaling by Multi-scale Modeling". Florida International University, Department of Physics, Miami, FL, March, 2017
3. "Multi-scale Modeling of Protein-protein Interactions for Understanding the Molecular Mechanisms of Cell adhesion and Signaling". University of South California, Department of Biological Sciences, Los Angeles, CA, February, 2016
4. "Multi-scale Modeling of Protein-protein Interactions for Understanding the Molecular Mechanisms of Cell adhesion and Signaling". Annual World Protein and Peptide Conference, Nan Jing, China, April, 2015
5. "Multi-scale Modeling of Protein-protein Interactions for Understanding the Molecular Mechanisms of Cell adhesion and Signaling". American Physical Society Annual Meeting, Denver, CO, March, 2014
6. "Multi-scale Modeling of Protein-protein Interactions for Understanding the Molecular Mechanisms of Cell adhesion and Signaling". Telluride Science Research Center, Telluride, CO, August, 2013
7. "Multi-scale Modeling of Protein-protein Interactions for Understanding the Molecular Mechanisms of Cell adhesion and Signaling". American Chemical Society Annual Meeting, New Orleans, LA, April, 2013
8. "Multi-scale Modeling of Protein-protein Interactions for Understanding the Molecular Mechanisms of Cell adhesion and Signaling". American Physical Society Annual Meeting, Baltimore, MD, March, 2013
9. "Multi-scale Studies of Cadherin-mediated Cell Adhesion". Fudan University, Department of Physics, Shanghai, China, June, 2012

10. "Multi-scale Studies of Cadherin-mediated Cell Adhesion". University of Kansas, Center of Bioinformatics, Lawrence, KS, March, 2012
11. "Multi-scale Studies of Cadherin-mediated Cell Adhesion". George Washington University, Department of Physics, Washington DC, February, 2012
12. "Multi-scale Studies of Cadherin-mediated Cell Adhesion". Northeastern University, Department of Biology, Boston, MA, February, 2012
13. "Multi-scale Studies of Cadherin-mediated Cell Adhesion". Georgia Institute of Technology, Department of Physics, Atlanta, GA, February, 2012
14. "Multi-scale Studies of Cadherin-mediated Cell Adhesion". Michigan State University, Department of Physics, East Lansing, MI, January, 2012
15. "Multi-scale Studies of Cadherin-mediated Cell Adhesion". Albert Einstein College of Medicine, Department of Systems and Computational Biology, Bronx, NY, January, 2012
16. "Multi-scale Studies of Cadherin-mediated Cell Adhesion". National Institute of Health, Bethesda, MD, December, 2011
17. "Multi-scale Simulations of Cadherin-mediated Cell Adhesion". New York Structural Biology Discussion Group Summer Meeting, Cold Spring Harbor, NY, August, 2011
18. "Multi-scale Simulations of Cadherin-mediated Cell Adhesion". Workshop: "from Computational Biophysics to Systems Biology", Julich Research Centre, Germany, July, 2011
19. "Multi-scale Simulations of Cadherin-mediated Cell Adhesion". University of Pennsylvania, Department of Biochemistry and Biophysics, Philadelphia, April, 2011
20. "Multi-scale Simulations of Cadherin-mediated Cell Adhesion". 55th Annual Meeting of Biophysical Society, Baltimore, March, 2011
21. "Multi-scale Simulations of Cadherin-mediated Cell Adhesion". University of California, San Francesco, Department of Pharmaceutical Chemistry, December, 2010
22. "Computational Study of Cadherin-mediated Junction Formation in Cell Adhesion". City University of New York, New York, September, 2010
23. "Prediction of Protein Domain Boundaries with SKELEFOLD". Columbia University, New York, 2007
24. "Prediction of Protein Tertiary Structures and Domain Boundaries with SKELEFOLD". University of California, San Francisco, 2007
25. "Prediction of Protein Tertiary Structures and Domain Boundaries with SKELEFOLD". University of Texas, Austin, 2007
26. "Exploring Subunit Motional Correlations in ATP Synthase Complex Using Elastic Normal Modes". FUDAN 95th Anniversary Celebration Symposium, Shanghai, China, May, 2000

Teaching Activities

1.	08/2018 – 10/2018	Introductions to Systems Biology	Albert Einstein College of Medicine
2.	03/2018 – 06/2018	Systems Biology Seminars	Albert Einstein College of Medicine
3.	08/2016 – 10/2016	Introductions to Systems Biology	Albert Einstein College of Medicine
4.	08/2014 – 10/2014	Introductions to Systems Biology	Albert Einstein College of Medicine
5.	02/2013 – 04/2013	Computational Biology of Proteins	Albert Einstein College of Medicine

Professional Experiences

1. **Grant Review Committee** of Proposal Evaluation for Allocation of Supercomputing Time for the Study of Molecular Dynamics Simulations on Anton 2, from National Academy of Sciences, DC, in August 2016
2. **Co-editor** of the book, named "Cell adhesion: From Molecular Biophysics to Cell Engineering" with *Springer*, the target publication date is June 2017
3. **Co-chair** of 8th Annual World Protein and Peptide Conference Platform Section: "Proteins: Dynamics, Stability, Aggregation, Metabolism and Degradation", in April, 2015
4. **Co-chair** of 55th Annual Meeting of Biophysical Society Platform Section: "Membrane receptor and signal transduction", in March, 2011
5. **Co-organizer** of the journal clubs for Applied Physics Program Research Fellows, Rice University, 2003-2004
6. **Co-founder** of the Fudan Bioinformatics Salon at Fudan University in 2000, and was invited to give an oral presentation at FUDAN 95th Anniversary Celebration Symposium, as the only student speaker
7. **Scientific reviewer** for Biophys. J., Protein Science, Structure, J. of Biomolecular Structure and Dynamics, J. of Chemical Information and Modeling, Journal of Bioinformatics and Comput. Biol., J. of Chemical Biol., BMC Bioinformatics, and others
8. **Member** of Biophysical Society, American Chemical Society (ACS), American Physical Society (APS), International Society of Computational Biology, Sigma Xi Scientific Research Society, Protein Society

Student/Postdoctoral Researchers Mentored

Current:

1.	Dr. Zhaoqian Su	Postdoctoral Fellow	02.2018-current
2.	Dr. Bo Wang	Postdoctoral Fellow	08.2017-current

Past:

1. Dr. Zhong-Ru Xie Postdoctoral Fellow 04.2013-07.2016
   Current Position:
   Assistant Professor, University of Georgia, School of Engineering
2. Dr. Jiawen Chen Postdoctoral Fellow 05.2013-11.2017
   Current Position:
   Associate Professor, Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences

Software Developed

1. **Ig BD Predictor:** a software to predict the homotypic binding status of Ig-Fold domain using multiple machine learning algorithms including support vector machine, random forest and back-propagation neural network
2. **PARC:** a software package in C++ and MATLAB that was developed to predict the kinetic rate of protein association
3. **Frag Pair Lib:** an interface fragment pair library was constructed from the current structure database of protein complexes
4. **Enzyme Simulator:** a simple FORTRAN program to study enzyme kinetics (Kinetic Monte-Carlo algorithm is used to simulate the diffusion-reaction process between enzymes and their substrates)
5. **OPUS-CA**: a knowledge-based potential used in protein tertiary structure prediction
6. **OPUS-DOM**: a program to predict protein domain boundaries

Technical Skills

- Genetic algorithms, Dynamic programming, Ant colony optimization, Agent-based modeling
- Neural networks, Self-organizing maps, Support vector machines, Voronoi Tessellation
- Fortran, C/C++, Mathematica, MatLab, Origin, CHARMM, GROMACS
- Knowledge-based potentials, SAXS-based structural Modeling, Homology modeling, threading