Jejoong Yoo

IBS Center for Self-assembly & Complexity
77 Cheongam-ro, Nam-gu
Pohang, 37672 Republic of Korea

Phone: +82 (054) 279-9952
Email: jejoong@gmail.com
Skype: jejoong.yoo.work

Current Position

Young Scientist Fellow (PI), Center for Self-assembly and Complexity, Institute for Basic Science

Education

University of Wisconsin-Madison **2005 – 2010**
Ph.D. in Biophysics on Dec. 24, 2010
Advisor: Prof. Qiang Cui
Thesis title: "Computational and Theoretical Studies of Lipid Membrane and Protein–Membrane Interactions"

Seoul National University, Seoul, Korea **1996 – 2001**
B.S. in Physics (Cum Laude)
B.S. in Molecular Biology (dual degree)

Research Achievements

Institute for Basic Science, Pohang, South Korea **2017 – present**
Young Scientist Fellow (PI), Center for Self-assembly and Complexity

- Developing a physics-based model of a whole nucleus.
- Discovering the phase separation mechanism of DNA and chromatin controlled by sequence and epigenetic modifications.

University of Illinois at Urbana-Champaign, IL **2010 – 2017**
Postdoctoral fellow, Department of Physics (Advisor: Prof. Aleksei Aksimentiev and Prof. Taekjip Ha)

- Developed a novel theory on the chemical and mechanical driving forces of chromatin organizations.
- Performed the first atomistic simulations of DNA origami and biomimetic DNA origami channels.
- Revealed the physics of DNA condensation using a large-scale atomistic simulation of DNA array.
- Developed chemically accurate intra- and inter-molecular force fields for protein, nucleic acids, lipid, and ions.
- Determined sequence-dependent energetics and dynamics of DNA loops through high-throughput computer simulations.

University of Wisconsin-Madison, Madison, WI **2005 – 2010**
Research Assistant, Department of Chemistry (Advisor: Prof. Qiang Cui)

- Studied arginine translocation mechanisms across lipid bilayers.
- Studied gating mechanisms of mechanosensitive channels using continuum mechanics, elastic network model and MD simulations.
- Studied effects of mechanical and chemical perturbations on the structure of lipid membranes.
- Analyzed local stress field at the protein-membrane interface in a membrane under stretching.

Korea Institute for Advanced Study, Seoul, Korea **2004 – 2005**
Research Assistant, Department of Computational Science (Advisor: Prof. Jooyoung Lee)

- Developed a knowledge-based scoring function of protein structures in preparation for the Critical Assessment of protein Structure Prediction (CASP6).
- In CASP6, in which I was one of two most active participants, our team was ranked 8th in non-homology target division among about 200 groups.

Employment

Corecess co., Ltd., Seoul, Korea **2002 – 2004**
Linux Device Driver Programmer

- Developed a multicasting service (e.g. Video on Demand) as a part of Linux kernel that ran on the network switch products of the company.

INZEN co., Ltd., Seoul, Korea **2001 – 2002**
Linux System/Network Programmer

- Developed UNIX server and client programs that collect information from security programs such as firewalls and manage those programs in a centralized way.

Samsung Advanced Institute of Technology, Seoul, Korea **Summer 2000**
Summer Intern, Bio Task Force Team

Awards

6. Young Scientist Fellowship (₩855,036,000 ∼ $750,000), Institute for Basic Science, 2017
5. $10,000 Pilot Project Award, University of Illinois at Urbana-Champaign, 2015
4. Post-Doctoral Research Fellowship from Center for the Physics of Living Cells, University of Illinois at Urbana-Champaign, 2010 – 2017
3. Superior Academic Performance, Seoul National University, 2000
2. Scholarship for Distinguished Undergraduates, Korea Foundation of Advanced Studies, 1998 – 1999
1. Superior Academic Performance, Seoul National University, 1996 – 1998

Publications

See my publications on Google Scholar | Scopus | PubMed | ResearchID | ResearchGate

34. Younghoon Kim, Jaehyoung Koo, In-Chul Hwang, Rahul Dev Mukhopadhyay, Soonsang Hong, Jejoong Yoo, Ajaz Dar, Ikjin Kim, Dohyun Moon, Tae Joo Shin, Young Ko & Kimoon Kim "Rational Design and Construction of Hierarchical Superstructures Using Shape-persistent Organic Cages: Porphyrin Box-based Metallosupramolecular Assemblies" ***Journal of the American Chemical Society***, 140:14547–14551, 2018 [Full text]
33. Hyunju Kang†, **Jejoong Yoo**†, Hong Soo Lee, Byeong-Kwon Sohn, Seung-Won Lee, Wenjie Ma, Jung-Min Kee, Aleksei Aksimentiev & Hajin Kim "Sequence-dependent DNA condensation as a driving force of DNA phase separation" ***Nucleic Acids Research***, 46:9401–9413, 2018 [Full text]
32. Alexander Ohmann, Chen-Yu Li, Christopher Maffeo, Kareem Al Nahas, Kevin N Baumann, Kerstin Göpfrich, **Jejoong Yoo**, Ulrich F Keyser & Aleksei Aksimentiev "A synthetic enzyme built from DNA flips 10^7 lipids per second in biological membranes" ***Nature Communications***, 9:2426, 2018 [Full text]
31. **Jejoong Yoo** & Aleksei Aksimentiev "New tricks for old dogs: Improving the accuracy of biomolecular force fields by pair-specific corrections to non-bonded interactions" ***Physical Chemistry Chemical Physics***, 20:8432–8449, 2018 [Full text]
30. Kyeng Min Park, Kangkyun Baek, Young Ho Ko, Annadka Shrinidhi, James Murray, Won Hyuk Jang, Ki Hean Kim, Jun-Seok Lee, **Jejoong Yoo**, Sungwan Kim & Kimoon Kim "Mono-allyloxylated Cucurbit[7]uril Acts as an Unconventional Amphiphile to Form Light-responsive Vesicles" ***Angewandte Chemie International Edition***, 57:3132–3136, 2018 [Full text]

29. **Jejoong Yoo** & Aleksei Aksimentiev "Refined Parametrization of Non-bonded Interactions Improves Conformational Sampling and Kinetics of Protein Folding Simulations" ***The Journal of Physical Chemistry Letters***, 7:3812–3818, 2016 [Full text]
28. Kerstin Göpfrich, Chen-Yu Li, Maria Ricci, Satya Prathyusha Bhamidimarri, **Jejoong Yoo**, Bertalan Gyenes, Alexander Ohmann, Mathias Winterhalter, Aleksei Aksimentiev & Ulrich F. Keyser "Large-Conductance Transmembrane Porin Made from DNA Origami" ***ACS Nano***, 10:8207–8214, 2016 [Full text]
27. Kerstin Göpfrich, Chen-Yu Li, Iwona Mames, Satya Prathyusha Bhamidimarri, Maria Ricci, **Jejoong Yoo**, Adam Mames, Alexander Ohmann, Mathias Winterhalter, Eugen Stulz, Aleksei Aksimentiev & Ulrich F. Keyser "Ion channels made from a single membrane-spanning DNA duplex" ***Nano Letters***, 16:4665–4669, 2016 [Full text]
26. Scott Michael Slone, Chen-Yu Li, **Jejoong Yoo** & Aleksei Aksimentiev "Molecular mechanics of DNA bricks: In situ structure, mechanical properties and ionic conductivity." ***New Journal of Physics***, 18:055012, 2016 [Full text]
25. **Jejoong Yoo**, James Wilson & Aleksei Aksimentiev "Improved model of hydrated calcium ion for molecular dynamics simulations using classical biomolecular force fields" ***Biopolymers***, 105:752–763, 2016 [Full text]
24. Swati Bhattacharya†, **Jejoong Yoo**† & Aleksei Aksimentiev "Water mediates recognition of DNA sequence via ionic current blockade in a biological nanopore." ***ACS Nano***, 10:4644–4651, 2016 [Full text]
23. Chris Maffeo, **Jejoong Yoo** & Aleksei Aksimentiev "De novo prediction of DNA origami structures through atomistic molecular dynamics simulation" ***Nucleic Acids Research***, 44:3013–3019, 2016 [Full text]
22. **Jejoong Yoo**†, Hajin Kim†, Aleksei Aksimentiev & Taekjip Ha "Direct evidence for sequence-dependent attraction between double-stranded DNA controlled by methylation" ***Nature Communications***, 7:11045, 2016 [Full text]
21. Thuy Ngo, **Jejoong Yoo**, Qing Dai, Qiucen Zhang, Chuan He, Aleksei Aksimentiev & Taekjip Ha "Effect of cytosine modifications on DNA flexibility and nucleosome mechanical stability" ***Nature Communications***, 7:10813, 2016 [Full text]
20. **Jejoong Yoo** & Aleksei Aksimentiev "The structure and intermolecular forces of DNA condensates" ***Nucleic Acids Research***, 44:2036–2046, 2016 [Full text]
19. **Jejoong Yoo** & Aleksei Aksimentiev "Improved parameterization of amine–carboxyate and amine–phosphate interactions for molecular dynamics simulations using the CHARMM and AMBER force fields" ***Journal of Chemical Theory and Computation***, 12:430–443, 2016 [Full text]
18. **Jejoong Yoo** & Aleksei Aksimentiev "Molecular dynamics of membrane-spanning DNA channels: Conductance mechanism, electro-osmotic transport and mechanical gating" ***The Journal of Physical Chemistry Letters***, 6:4680–4687, 2015 [Full text]
17. Chen-Yu Li, Elisa A. Hemmig, Jinglin Kong, **Jejoong Yoo**, Silvia Hernández-Ainsa, Ulrich F. Keyser & Aleksei Aksimentiev "Ionic conductivity, structural deformation and programmable anisotropy of DNA origami in electric field." ***ACS Nano***, 9:1420–1433, 2015 [Full text]
16. Chris Maffeo, **Jejoong Yoo**, Jeffrey Comer, David Wells, Binquan Luan & Aleksei Aksimentiev "Close encounters with DNA." ***J. Phys.: Condens. Matter***, 26:413101, 2014 [Full text]
15. **Jejoong Yoo** & Aleksei Aksimentiev "In situ structure and dynamics of DNA origami determined through molecular dynamics simulations." ***Proceedings of the National Academy of Sciences***, 110:20099–20104, 2013. [Full text]

14. **Jejoong Yoo**, Meyer Jackson & Qiang Cui "A comparison of coarse-grained and continuum models for membrane bending in lipid bilayer fusion pores." ***Biophysical Journal***, 104:841–852, 2013. [Full text]
13. **Jejoong Yoo** & Qiang Cui "Membrane-mediated protein-protein interactions and connection to elastic models: a coarse-grained simulation analysis of gramicidin A association." ***Biophysical Journal***, 104:128–138, 2013. (Cover) [Full text]
12. **Jejoong Yoo** & Qiang Cui "Three-dimensional stress field around a membrane protein: atomistic and coarse-grained simulation analysis of gramicidin A." ***Biophysical Journal***, 104:117–127, 2013. [Full text]
11. Chris Maffeo, Swati Bhattacharya, **Jejoong Yoo**, David Wells & Aleksei Aksimentiev "Modeling and simulation of ion channels." ***Chemical Reviews***, 112:6250–6284, 2012. (Cover) [Full text]
10. **Jejoong Yoo** & Aleksei Aksimentiev "Competitive binding of cations to duplex DNA revealed through molecular dynamics simulations." ***The Journal of Physical Chemistry B***, 43:12946–12954, 2012. [Full text]
9. **Jejoong Yoo** & Aleksei Aksimentiev "Improved parametrization of Li^+, Na^+, K^+, and Mg^{2+} ions for all-atom molecular dynamics simulations of nucleic acid systems." ***The Journal of Physical Chemistry Letters***, 3:45–50, 2012. [Full text]
8. **Jejoong Yoo** & Qiang Cui "Chemical versus mechanical perturbations on the protonation state of arginine in complex lipid membranes: insights from microscopic pK_a calculations." ***Biophysical Journal***, 99:1529–1538, 2010. [Full text]
7. **Jejoong Yoo** & Qiang Cui "Curvature generation and pressure profile modulation in membrane by lysolipids: Insights from Coarse-Grained Simulations." ***Biophysical Journal***, 97:2267–76, 2009. [Full text]
6. Yuye Tang, Xi Chen, **Jejoong Yoo**, Arun Yethiraj & Qiang Cui "Numerical simulation of nanoindentation and patch clamp experiments on mechanosensitive channels of large conductance in escherichia coli." ***Exp. Mech.***, 49(1): 35–46, 2009. [Full text]
5. **Jejoong Yoo** & Qiang Cui "Does arginine remain protonated in the lipid membrane? Insights from microscopic pK_a calculations." ***Biophysical Journal***, 94, L61–L63, 2008. [Full text]
4. Xi Chen, Qiang Cui, Yuye Tang, **Jejoong Yoo** & Arun Yethiraj "Gating mechanisms of mechanosensitive channels of large conductance, I: a continuum mechanics-based hierarchical framework." ***Biophysical Journal***, 95:563–580, 2008. (Cover) [Full text]
3. Yuye Tang, **Jejoong Yoo**, Arun Yethiraj, Qiang Cui & Xi Chen "Gating mechanisms of mechanosensitive channels of large conductance, II: systematic study of conformational transitions." ***Biophysical Journal***, 95:581–596, 2008. [Full text]
2. Yuye Tang, **Jejoong Yoo**, Arun Yethiraj, Qiang Cui & Xi Chen "Mechanosensitive channels: insights from continuum-based simulations." ***Cell Biochem. Biophys.***, 52:1–18, 2008. [Full text]
1. Yuye Tang, Guoxin Cao, Xi Chen, **Jejoong Yoo**, Arun Yethiraj & Qiang Cui "A finite element framework for studying the mechanical response of macromolecules: application to the gating of the mechanosensitive channel MscL." ***Biophysical Journal***, 91:1248–1263, 2006. (Cover) [Full text]

† Equal Contribution; ∗ Corresponding author

Book Chapters

1. **Jejoong Yoo**, Chen-Yu Li, Scott Michael Slone, Christopher Maffeo & Aleksei Aksimentiev "A Practical Guide to Molecular Dynamics Simulations of DNA Origami Systems." ***DNA Nanotechnology***, pp 209–229, 2018 `[Full text]`

Invited talks

36. Arctic Biophysics Meeting on Epigenetics and Chromosome Dynamics, 2019, "Epigenetic Principles for Programming Extreme Bendability of DNA"
35. 2019 Conference of the Federation of Korean Societies for Biomolecular Sciences, 2019, "Programming Extreme Bendability of DNA Using Epigenetic Principles"
34. The 18th KIAS Conference on Protein Structure and Function, 2018, "Molecular dynamics simulations using accurate charge-charge interactions predict unexpected phase behaviors of dna controlled by epigenetic modifications"
33. DGIST, 2018, "Cracking the Natures Programming Manual for Mechanical Looping and Phase Separation of DNA"
32. Korean Physical Society Meeting, 2018, "Computer-Aided Design of Biomimetic DNA Channels"
31. APCTP Biophysics summer school, 2018, ""
30. Fourth Polish-Korean Conference entitled "Protein Folding: Theoretical and Experimental Approaches", 2018, "Refined parametrization of the CHARMM and AMBER force fields for protein folding and protein-DNA interactions"
29. GIST, 2018, ""
28. Korean Physical Society Meeting, 2018, "Epigenetically controlled phase separation of DNA revealed by multi-scale simulations and experiments"
27. POSTECH Human chromosome, 2018, "..."
26. 3rd International Symposium on Mechanobiology, 2017, "Mechanical forces of DNA looping and condensation revealed by high-throughput computer simulations and single-molecule experiments"
25. Bio-Complex seminar series, Department of Physics, POSTECH, 2017
24. Korean Chemical Society Meeting, 2017
23. NYU, Department of Chemistry, 2017 "The Physics of Chromosome: From DNA Loops to Nucleus-Scale Structures"
22. Biophysical Society Meeting, Molecular Biophysics Subgroup, 2017 "High throughput simulations reveal how sequence and methylation control DNA looping and self-association"
21. Virginia Tech, Department of Physics, 2017 "The Physics of Chromosome: From DNA Loops to Nucleus-Scale Structures"
20. Institute for Basic Science, 2016 "Molecular Driving Forces in the Self-assembly of Chromosomes and DNA Nano-machines"
19. Sungkyunkwan University, Department of Chemistry, 2016 "Molecular Driving Forces in the Self-assembly of Chromosomes and DNA Nano-machines"
18. 3rd Molecular Simulation Summer School, University of Calgary, 2016 "DNA origami tutorial"
17. 4th Midwest Single Molecule Workshop, University of Iowa, 2016 "Toward a physical energy landscape of epigenetics"
16. Blue Waters Symposium, 2016 "Improved Molecular Dynamics Model Suggests Novel Epigenetic Mechanisms"
15. Michigan Technological University, Department of Physics, 2016 "A novel epigenetic mechanism of DNA compaction and Atomistic simulations of DNA origami"
14. Korea Institute for Advanced Study (KIAS), 2016 "A novel epigenetic mechanism of DNA compaction and atomistic simulations of DNA origami"
13. Ulsan National Institute of Science and Technology (UNIST), 2016 "A novel epigenetic mechanism of DNA compaction and atomistic simulations of DNA origami"

12. University of Tennessee, Knoxville, Department of Chemistry, 2016 "A novel epigenetic mechanism of DNA compaction and atomistic simulations of DNA origami"
11. North Carolina State University, Department of Physics, 2016 "A novel epigenetic mechanism of DNA compaction and atomistic simulations of DNA origami"
10. Arizona State University, Department of Physics, 2016 "A novel epigenetic mechanism of DNA compaction and atomistic simulations of DNA origami"
9. University of Illinois at Urbana-Champaign, CSE Fall 2014 Seminar Series, 2014 "DNA senses the sequence of neighbors"
8. Seoul National University, Department of Chemical Engineering, 2014
7. Blue Waters Symposium, 2014
6. Ulsan National Institute of Science and Technology (UNIST), 2014
5. CPLC Student/Postdoctoral Fellow Symposium, 2013
4. Korea Institute for Advanced Study (KIAS), 2012
3. CPLC Student/Postdoctoral Fellow Symposium, 2012
2. CPLC at UIUC, 2010
1. Student Addendum Conference in Sixth meeting on the critical assessment of techniques for protein structure prediction, 2004

Presentations

9. Biophysical Society Meeting, 2016
8. The 21st International Conference on DNA Computing and Molecular Programming (DNA21), 2015
7. Gordon Conference on Chromatin Structure and Function, 2014
6. Midwest Chromatin Meeting, 2014
5. Biophysical Society Meeting, 2014
4. Biophysical Society Meeting, 2012
3. Chromatin Meeting, 2011
2. American Chemical Society Meeting, 2007
1. American Conference on Theoretical Chemistry, 2007

Web applications

- Cadnano2PDB, `https://nanohub.org/resources/cadnanocvrt`, automatically converts a DNA origami design file to atomic structure and MD simulation input files.

Services

- Reviewer of the Journal of Physical Chemistry
- Reviewer of Biophysical Chemistry

Computer Skills

- Experts in molecular dynamics packages (10 years): Gromacs, CHARMM, NAMD, and Anton.
- Experienced in C programming in UNIX/Linux environment (8 years): system, network, Linux device driver, MPI, multi threads etc.
- Fluent in programming languages (14 years): C and Perl
- Experienced in Fortran, JAVA and PHP
- Experienced in Matlab programming
- Experienced in web programming using PHP and MySQL

References

- **Prof. Qiang Cui**
  Department of Chemistry
  Boston University
  590 Commonwealth Avenue
  Boston, MA 02215-2521
  qiangcui@bu.edu
- **Prof. Aleksei Aksimentiev**
  Department of Physics
  University of Illinois at Urbana-Champaign
  1110 West Green Street
  Urbana, IL 61801-3080
  (217) 333-6495
  aksiment@illinois.edu
- **Prof. Taekjip Ha**
  Department of Biophysics and Biophysical Chemistry
  Johns Hopkins University School of Medicine
  725 N. Wolfe St., 703 WBSB
  Baltimore, MD 21205
  tjha@jhu.edu