Pengzhi Zhang, Ph.D.

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Professional experience

2022 – present, Research associate, Houston Methodist Research Institute
Conduct research projects.

2019 – 2021, Research scientist, Department of Physics, University of Houston
Provide technical expertise to facilitate the design, implementation, and analysis of research procedures, techniques, and results, which enables investigators to conduct research projects.

- Applied machine learning models for fast prediction of *ab initio* atomic charges for calcium ions.
- Contributed to development of scientific software CTRAMER for interfacial charge transfer rates.
- Developed polarizable force fields for organic photovoltaic compounds and biological molecules.
- Processed mass spectrometry data with in-house and existing software programs.
- Planned for the data management including scientific data and in-house codes.
- Wrote research proposals for computational resources.
- Supervised junior members in the laboratory.

2017 – 2019, Research scientist, Research Computing Data Core, University of Houston
Offered researchers in a campus-wide community with training on high-performance computing (HPC) and one-on-one consultation to enhance their research with HPC by improving performance of their codes, as well as searching and implementing new algorithms.

- Supported researchers by profiling/debugging/optimizing computer codes.
- Developed/recommended workflows for computation on HPC clusters.
- Participated in writing research proposals.
- Participated in setting up exposition booths and prepared demonstration at national conferences.
- Assisted in organizing a conference about data science in health care and oil & gas industry.

2011 – 2017, Doctoral graduate student, Department of Physics, University of Houston
Advisor: Dr. Margaret S. Cheung, Pacific Northwest National Laboratory

- Investigated biological physics of protein association and regulation on synaptic plasticity.
- Established a theory of effects on a light-harvesting molecular triad by induced polarization.

Education

- Ph.D. in Physics, University of Houston, Houston, Texas — August, 2016
- M.S. in Physics, University of Houston, Texas — May, 2014
- B.S. in Physics, University of Science and Technology of China, Hefei, China — June, 2010

Publications

1. Tinnin J, Bhandari S, **Zhang P**, Geva E, Dunietz BD, Sun X, Cheung MS. “Linking Molecular and Quantum Phenomena to Charge-Transfer Differences in the DBP/C_{70} Organic Photovoltaic System”. *J. Phys. Chem. Lett.* (2022); 13, 763. doi: 10.1021/acs.jpclett.1c03618

2. Nde J, **Zhang P**, Ezerski JC, Lu W, Knapp K, Wolynes, PG, Cheung MS. "Coarse-Grained Modeling and Molecular Dynamics Simulations of Ca^{2+}-Calmodulin". *Front. Mol. Biosci.* (2021); 8, 753. doi: 10.3389/fmolb.2021.661322
3. Tinnin J, Aksu H, Tong Z, **Zhang P**, Geva E, Dunietz BD, Sun X, Cheung MS. "CTRAMER: An Open-source Software Package for Correlating Interfacial Charge Transfer Rate Constants with Donor / acceptor Geometries in Organic Photovoltaic Materials". *J Chem Phys*. (2021); 154, 214108. doi: 10.1063/5.0050574
4. **Zhang P**, Han J, Cieplak P, Cheung MS. "Determining the Atomic Charge of Calcium Ion Requires the Information of Its Coordination Geometry in an EF-hand Motif". *J Chem Phys.* (2021); 154, 124104. doi: 10.1063/5.0037517
5. Han J, **Zhang P**, Aksu H, Maiti B, Sun X, Geva E, Dunietz BD, Cheung MS. "On the Interplay between Electronic Structure and Polarizable Force Fields When Calculating Solution-Phase Charge-Transfer Rates". *J Chem Theory Comput*. (2020);16, 6481-6490. doi:10.1021/acs.jctc.0c00796
6. Ezerski JC, **Zhang P**, Jennings NC, Waxham MN, Cheung MS. "Molecular Dynamics Ensemble Refinement of Intrinsically Disordered Peptides According to Deconvoluted Spectra from Circular Dichroism". *Biophys J*. (2020);118,1665-1678. doi:10.1016/j.bpj.2020.02.015
7. Tinnin J, Bhandari S, **Zhang P**, Aksu H, Maiti B, Geva E, Dunietz BD, Sun X, Cheung MS. "Molecular Level Exploration of the Structure-Function Relations Underlying Interfacial Charge Transfer in the Subphthalocyanine/ C_{60} Organic Photovoltaic System". *Phys Rev Appl*. (2020);13, 1. doi:10.1103/PhysRevApplied.13.054075
8. Sun X, **Zhang P**, Lai Y, Williams KL, Cheung MS, Dunietz BD, Geva E. "Computational Study of Charge-Transfer Dynamics in the Carotenoid-Porphyrin-C_{60} Molecular Triad Solvated in Explicit Tetrahydrofuran and Its Spectroscopic Signature". *J Phys Chem C*. (2018);122, 11288-11299. doi:10.1021/acs.jpcc.8b02697
9. Starovoytov ON, **Zhang P**, Cieplak P, Cheung MS. "Induced Polarization Restricts the Conformational Distribution of a Light-harvesting Molecular Triad in the Ground State". *Phys Chem Chem Phys*. (2017);19, 22969-22980. doi:10.1039/c7cp03177g
10. **Zhang P**, Tripathi S, Trinh H, Cheung MS. "Opposing Intermolecular Tuning of Ca^{2+} Affinity for Calmodulin by Neurogranin and CaMKII Peptides". *Biophys J*. (2017);112, 1105-1119. doi:10.1016/j.bpj.2017.01.020
    - Cover of the issue
    - Recommended by Uversky V in *Faculty Opinions*. doi: 10.3410/f.727458175.793534435
11. Tripathi S, Wang Q, **Zhang P**, Hoffman L, Waxham MN, Cheung MS. "Conformational Frustration in Calmodulin-target Recognition". *J Mol Recognit*. (2015);28, 74-86. doi:10.1002/jmr.2413
12. *Wang Q, ***Zhang P**, Hoffman L, Tripathi S, Homouz D, Liu Y, Waxham MN, Cheung MS. "Protein Recognition and Selection Through Conformational and Mutually Induced Fit". *Proc Natl Acad Sci U S A*. (2013);110, 20545-20550. doi:10.1073/pnas.1312788110.
    * Equal authorship

Manuscript in preparation / submitted

- Jennings NC, Cieplak P, Cheung MS, **Zhang P**. "Network Theory Aided Machine Learning for Atomic Charges of Ca^{2+} in Ca^{2+} Binding Proteins". *To be submitted soon.*

Peer reviewer

- Biophysical Journal
- Scientific Reports
- Physical Chemistry Chemical Physics

Oral presentations

- "Opposing Intermolecular Tuning of Ca^{2+} Affinity for Calmodulin by Neurogranin and CaMKII Peptides", Texas Section of the American Physical Society, Houston, TX, 2018
- "Modeling of Binding of Calmodulin and Intrinsically Disordered Peptide Neurogranin", Supercomputing 14 Exposition session, New Orleans, LA, 2014
- "Coarse-grained Molecular Simulation of Calmodulin-target Interactions", American Physical Society Annual Meeting, Baltimore, MD, 2013
- "How Calmodulin Binds to Its Targets", Supercomputing 12 Exposition session, Salt Lake City, UT, 2012

Poster presentations

- "Rapid Determination of Ca^{2+} Charge in Varying Calmodulin Environments Using Machine Learning", Annual Southwest Theoretical and Computational Chemistry Meeting, Norman, OK, 2019
- "Intermolecular Interaction between Calmodulin and Intrinsically Disordered Protein Neurogranin Alters Calcium Binding", Sealy Center for Structural Biology and Molecular Biophysics Symposium, Galveston, TX, 2015
- "Protein recognition and selection through conformational and mutually induced fit", Sealy Center for Structural Biology and Molecular Biophysics Symposium, Galveston, TX, 2014
- "Protein Recognition and Selection Through Conformational and Mutually Induced-fit", Biophysical Society Annual Meeting, San Francisco, CA, 2014

Grants writing

- Determination of Calcium Charge in Varying Calmodulin Environments Using Machine Learning
  Extreme Science and Engineering Discovery Environment (XSEDE: TG-MCB190109)
  Role: PI
- Post-Marcus Theory & Simulation of Interfacial Charge Transfer in Organic Semiconducting Materials
  National Energy Research Scientific Computing Center (NERSC)
  Role: co-PI
- Principles for Tuning Target Selectivity in Signaling Proteins
  National Institute of Health (NIH: 2R01GM097553)
  Role: participation in proposal writing and provided preliminary results

References

Available upon request.