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Education

2015-2022	Ph.D of Chemistry. *Boston University, USA.* Graduation : 2022/1/25
2013-2015	B.S. of Chemistry. *Temple University, Philadelphia, USA.* Graduation : 2015/5/8
2011-2013	A.S. of Science. *Community College of Philadelphia, Philadelphia, USA.* Graduation : 2013/5/4

Honors

2019	Lichtin Award for Excellence in Research.
2018	RIKEN Short-Term International Program Associate.
2017	NSF GROW/JSPS Fellow.
2015-2020	NSF Graduate Research Fellowship.
2015	PECO Scholar, *PECO*.
2015	Feynman Memorial Scholar, *Temple University*.
2014	Diamond Scholar Summer Fellow, *Temple University*.
2013	NSF Research Experience for Undergraduates, *Boston University*.

Service and Teaching

2018-2019	Teaching Fellow, Boston University CH225 - Mathematical Methods for Chemists.
2016-2018	Graduate Fellowships Mentorship and Workshops, Boston University Chemistry Department.
2015-2016	Writing Mentor, Boston University Chemical Writing Program.
2015-2016	High School Science Outreach Instructor, Boston University Women in Chemistry.
2014-2015	Science Instructor, TeenSHARP.

Presentations 2015-

2023 "Parameterization of a sequence-specific coarse-grained collagen model," *Biophysical Society Annual Meeting (Poster).*

2022 "Simulating Atomistic Structure of Collagen : Force Field Corrections and Beyond," *Protein Folding Dynamics Gordon Research Conference (Poster).*

2022 "Atomistic Structure of Collagen : Validation of Atomistic Force Fields," *Boston University Physical Chemistry Lecture Series (Talk).*

2022 "Developing a chemically-defined coarse-grained force field for extracellular Matrix simulations," *Pacifichem (Virtual Poster).*

2021 "Intrinsically disordered membrane protein amyloid precursor protein C99 domain conformational ensemble and complex solvation with cholesterol," *Pacifichem (Virtual Talk).*

2020 "Exploring APP-C99 complexes in lipid bilayers and their role in Alzheimer's disease," *ACS Annual Meeting, Philadelphia (Virtual Poster).*

2019 "Phase separations in lipid membranes, what they have to do with proteins, and recent developments in MD-based modeling," *Boston University Physical Chemistry Lecture Series (Talk).*

2019 "Probing the roles of membrane and cholesterol on Aβ biogenesis and toxicity," *ACS Annual Meeting, Orlando (Talk).*

2018 "Understanding an Intrinsically Disordered Membrane Protein in Alzheimer's Disease via Molecular Simulation," *RIKEN Summer School (Poster) ; Computational Biophysics at the Molecular and Meso Scales, ICISE Vietnam (Talk).*

2017 "Structure of APP-C99 1-99 and Implications for its Role in Amyloidogenesis," *Kyoto University (Talk).*

2017 "Role of cholesterol in ternary lipid membrane phase separation observed via coarse-grained simulations," *American Theoretical Chemistry Conference (Poster) ; Japanese Biophysical Society (Poster).*

2017 "Tempering in OpenMM and GENESIS," *Temple University Current Trends in Molecular Dynamics Software Design Workshop (Poster).*

2017 "Critical investigation of finite size and cholesterol effects in lipid domain formation," *RIKEN, Wako-shi (Talk) ; Boston University Chemistry Student Graduate Seminar Series ; Nagoya University IGER Seminar Series (Talk).*

2016 "Exploring phase separation and domain formation in lipid bilayers through molecular simulation," *Boston University Graduate Research Symposium ; ACS National Meeting, Philadelphia (Poster).*

2015 "Examining the conformational dynamics of the N-terminal region of mdm2 using markov state model approaches," *ACS National Meeting, Boston (Poster).*

2015 "Microsecond simulations of mdm2 and its complex with p53 yield insight into force field accuracy and conformational dynamics," *Temple University Undergraduate Research Forum and Creative Works Symposium (Talk).*

Publications

20. "Characterizing the transmembrane domains of ADAM10 and BACE1 and the impact of membrane composition" C. Abraham, L. Xu, **G.A. Pantelopulos**, J.E. Straub, *Biophys. J.* Submitted (2023)
19. "MolPainter : A Tool for Painting and Solvating Layered Molecular Systems" **G.A. Pantelopulos** , A. Liberatore, *J. Open Source Softw.* Accepted (2023)
18. "Formation of extramembrane β-strands controls dimerization of transmembrane helices in amyloid precursor protein C99" **G.A. Pantelopulos**, D. Matsuoka, J.M. Hutchison, C.R. Sanders, Y. Sugita, J.E. Straub, D. Thirumalai, *Proc. Natl. Acad. Sci. USA* **119**, 52 (2023)
17. "Efficient calculation of the free energy for protein partitioning using restraining potentials," S. Kwon, **G.A. Pantelopulos**, J.E. Straub, *Biophys. J.* **122**, 1 (2023)
16. "Finite-size effects and optimal system sizes in simulations of surfactant micelle self-assembly," J. Harris, **G.A. Pantelopulos**, J.E. Straub, *J. Phys. Chem. B* **19**, 125 (2021)
15. "Direct Observation of Cholesterol Dimers and Tetramers in Lipid Bilayers," M.R. Elkins, A. Bandara, **G.A. Pantelopulos**, J.E. Straub, M. Hong, *J. Phys. Chem. B* **7**, 125 (2021)
14. "Impact of Cholesterol Concentration and Lipid Phase on Structure and Fluctuation of Amyloid Precursor Protein," **G.A. Pantelopulos**, A. Panahi, J.E. Straub, *J. Phys. Chem. B* **45**, 124, (2020)
13. "Bicelles Rich in both Sphingolipids and Cholesterol and Their Use in Studies of Membrane Proteins," J. Hutchinson, K. Shih, H. Scheidt, S. Fantin, **G.A. Pantelopulos**, H. Harrington, K. Mittendorf, S. Qian, R. Stein, S. Collier, M. Chambers, J. Kastaras, M. Voehler, B. Ruotolo, D. Huster, R. McFeeters, J. Straub, M. Neih, C. Sanders *J. Am. Chem. Soc.*, **29**, 142 (2020)
12. "Exploring the impact of line tension on the spatial localization of protein in phase-separated lipid bilayers," A. Bandara, A. Panahi, **G.A. Pantelopulos**, T. Nagai, J. E. Straub, *J. Phys. Chem. B*, **20**, 204702 (2019)
11. "Aerosol-OT Surfactant Forms Stable Reverse Micelles in Aploar Solvent in the Absence of Water," R. Urano, **G.A. Pantelopulos**, J. E. Straub, *J. Chem. Phys.* **14**, 149 (2019).
10. "Structural Role of Cholesterol in Complex Lipid Bilayer Phases Observed via MD Simulation," **G.A. Pantelopulos**, J. E. Straub, *Biophys. J.* **115**, 2167-2178 (2018).
9. "Characterization of dynamics and mechanism in the self-assembly of AOT reverse micelles," R. Urano, **G.A. Pantelopulos**, S. Song, J. E. Straub, *J. Chem. Phys.* **14**, 144901 (2018).
8. "Structure of APP-C99_{1-99} and Implications for Role of Extra-Membrane Domains in Function and Oligomerization," **G.A. Pantelopulos**, J. E. Straub, D. Thirumalai, Y. Sugita, *Biochim. Biophys. Acta - Biomembranes* **1860**, 1698-1708 (2018).
7. "Critical size dependence of domain formation observed in coarse-grained simulations of bilayers composed of ternary lipid mixtures," **G.A. Pantelopulos**, T. Nagai, A. Bandara, A. Panahi, J. E. Straub, *J. Chem. Phys.* **147** 095101 (2017).
6. "Bridging microscopic and macroscopic mechanisms of p53-MDM2 binding using molecular simulations and kinetic network models," G. Zhou, **G.A. Pantelopulos**, S. Mukherjee, V. Voelz, *Biophys. J.* **113**, 785-793 (2017).
5. "Exploring the structure and stability of cholesterol dimer formation in multicomponent lipid bilayers," A. Bandara, A. Panahi, **G.A. Pantelopulos**, J.E. Straub *J. Comp. Chem.* **38**, 1479-1488 (2016).
4. "Specific binding of cholesterol to C99 domain of Amyloid Precursor Protein depends critically on charge state of protein," A. Panahi, A. Bandara, **G.A. Pantelopulos**, L. Dominguez and J.E. Straub, *J. Phys. Chem. Lett.* **7**, 3535-3541 (2016).
3. "On the use of mass scaling for stable and efficient simulated tempering with molecular dynamics," T. Nagai, **G.A. Pantelopulos**, T. Takahashi, J.E. Straub *J. Comp. Chem.* **37** 2017-2028 (2016).
2. "Markov models of the apo-MDM2 lid region reveal diffuse yet two-state binding dynamics and receptor poses for computational docking," S. Mukherjee, **G.A. Pantelopulos**, V.A. Voelz *Sci. Rep.* **6** 31631 (2016).
1. "Microsecond simulations of mdm2 and its complex with p53 yield insight into force field accuracy and conformational dynamics," **G.A. Pantelopulos**, S. Mukherjee, V.A. Voelz, *Proteins* **83** 1665-1676 (2015).