George A. PANTELOPULOS

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1991 May 28 Birthdate

USA Nationality

Single with no children

Graduate Student

Education

2015-Current Ph.D of Chemistry. *Boston University, USA*.

Expected Graduation: 2020/5/19

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

2018 RIKEN SHORT-TERM INTERNATIONAL PROGRAM ASSOCIATE.

2017 NSF GROW/JSPS Fellow.

2015-Current NSF GRADUATE RESEARCH FELLOWSHIP.

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 Me-

THODS FOR CHEMISTS.

2016-2018 Graduate Fellowships Mentorship and Workshops, Boston Univer-

SITY CHEMISTRY DEPARTMENT.

2015-2016 Writing Mentor, Boston University Chemical Writing Program.

2015-2016 HIGH SCHOOL SCIENCE OUTREACH INSTRUCTOR, BOSTON UNIVERSITY WO-

MEN IN CHEMISTRY.

2014-2015 Science Instructor, TeenSHARP.

Presentations

2019	"Probing the roles of membrane and cholesterol on $A\beta$ 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 Amy- Loidogenesis," <i>Kyoto University (Talk)</i> .
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 li- pid domain formation," RIKEN, Wako-shi (Talk); Boston University Che- mistry 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).
2014-2015	"MICROSECOND SIMULATIONS OF MDM2 AND ITS COMPLEX WITH P53 YIELD INSIGHT INTO FORCE FIELD ACCURACY AND CONFORMATIONAL DYNAMICS," ACS Philadelphia Younger Chemists Committee Conference (Poster); Emory STEM Research Symposium (Poster).
2013-2014	"Molecular Dynamics Simulations of the P53-MDM2 Binding Interface," ACS Philadelphia Younger Chemists Committee Conference (Poster); ACS 248th National Meeting (Poster).

Publications

- * \equiv First author or equal to first author contributions
- 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, Accepted* (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-C99₁₋₉₉ 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).