

George A. PANTELOPULOS

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1991 May 28 Birthdate

USA Nationality

Single with no children

Graduate Student

## Education

<b>2015-Current</b>	PH.D OF CHEMISTRY. <i>Boston University, USA.</i> Expected Graduation : 2020/9/25
<b>2013-2015</b>	B.S. OF CHEMISTRY. <i>Temple University, Philadelphia, USA.</i> Graduation : 2015/5/8
<b>2011-2013</b>	A.S. OF SCIENCE. <i>Community College of Philadelphia, Philadelphia, USA.</i> Graduation : 2013/5/4

## Honors

<b>2019</b>	LICHTIN AWARD FOR EXCELLENCE IN RESEARCH.
<b>2018</b>	RIKEN SHORT-TERM INTERNATIONAL PROGRAM ASSOCIATE.
<b>2017</b>	NSF GROW/JSPS FELLOW.
<b>2015-Current</b>	NSF GRADUATE RESEARCH FELLOWSHIP.
<b>2015</b>	PECO SCHOLAR, <i>PECO</i> .
<b>2015</b>	FEYNMAN MEMORIAL SCHOLAR, <i>Temple University</i> .
<b>2014</b>	DIAMOND SCHOLAR SUMMER FELLOW, <i>Temple University</i> .
<b>2013</b>	NSF RESEARCH EXPERIENCE FOR UNDERGRADUATES, <i>Boston University</i> .

## Service and Teaching

<b>2018-2019</b>	TEACHING FELLOW, BOSTON UNIVERSITY CH225 - MATHEMATICAL METHODS FOR CHEMISTS.
<b>2016-2018</b>	GRADUATE FELLOWSHIPS MENTORSHIP AND WORKSHOPS, BOSTON UNIVERSITY CHEMISTRY DEPARTMENT.
<b>2015-2016</b>	WRITING MENTOR, BOSTON UNIVERSITY CHEMICAL WRITING PROGRAM.
<b>2015-2016</b>	HIGH SCHOOL SCIENCE OUTREACH INSTRUCTOR, BOSTON UNIVERSITY WOMEN IN CHEMISTRY.
<b>2014-2015</b>	SCIENCE INSTRUCTOR, TEENSHARP.

## Presentations

- 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 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 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)*.
- 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

20. "MolPainter and MolSolvator : tools for drawing and solvating complex planar molecular systems of arbitrary composition and molecule placement," **G.A. Pantelopulos\***, A. Liberatore, *In Preparation*, (2020)
19. "Evaluation and applicability of prominent coarse-grained models of cholesterol in molecular dynamics simulation." **G.A. Pantelopulos\***, A. Bandara, J.E. Straub, *In Preparation*, (2020)
- 18 "Characterization of the intrinsically disordered monomer and homodimer of APP-C99 1-99" **G.A. Pantelopulos\***, J. Hutchinson, D. Matsuoka, C. Sanders, Y. Sugita, J.E. Straub, *In Preparation*, (2020)
17. "De novo all-atom molecular dynamics simulation of amyloid precursor protein in phase separating ternary lipid mixture." **G.A. Pantelopulos\***, A. Bandara, J.E. Straub, *In Preparation*, (2020)
15. "Cholesterol effects amyloid precursor protein via the liquid ordered phase as a nonbinding solvent." **G.A. Pantelopulos\***, A. Panahi, J.E. Straub, *In Preparation*, (2020)
14. "Direct Observation of Cholesterol Dimers and Tetramers in Lipid Bilayers," M.R. Elkins, A. Bandara, **G.A. Pantelopulos**, J.E. Straub, M. Hong, *Submitted* (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.*, *Accepted* (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 Apolar 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<sub>1-99</sub> 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).