

George A. PANTELOPULOS

Laboratory of Chemical Physics

NIH-NIDDK

Bethesda, MD, USA

Phone : +1 (302) 419-7373 (cell)

Email : [george.pantelopulos@nih.gov](mailto:george.pantelopulos@nih.gov)

1991 May 28 Birthdate

USA Nationality

Single with no children

## 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

- 2021** “DEVELOPING A CHEMICALLY-DEFINED COARSE-GRAINED FORCE FIELD FOR EXTRACELLULAR MATRIX SIMULATIONS,” *Pacificchem (Virtual Poster)*.
- 2021** “INTRINSICALLY DISORDERED MEMBRANE PROTEIN AMYLOID PRECURSOR PROTEIN C99 DOMAIN CONFORMATIONAL ENSEMBLE AND COMPLEX SOLVATION WITH CHOLESTEROL,” *Pacificchem (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 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

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 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).