George A. PANTELOPULOS

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Boston, MA, USA

USA Nationality

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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.

2015 PECO Scholar.

2015 FEYNMAN MEMORIAL SCHOLAR.

2014-2015 UNDERGRADUATE RESEARCH FELLOW, Temple University.
2014 DIAMOND SCHOLAR SUMMER FELLOW, Temple University.

2013 NSF RESEARCH EXPERIENCE FOR UNDERGRADUATES, Boston University.

Service and Teaching

2018 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.

2013 Chemistry Tutor, Community College of Philadelphia.

Extracurricular Training

2017 FRONTEIRS IN COMPUTATIONAL BIOPHYSICS AND BIOCHEMISTRY, RIKEN,

Japan.

2016 ERICE SCHOOL: EXPLORING AND QUANTIFYING ROUGH FREE ENERGY

Landscapes, International School of Statistical Physics, Ettore Majorana

Foundation and Centre for Scientific Culture, Erice, Sicily, Italy.

2015 Alan Alda Communicating Science Workshop, Boston University, USA.

2015 School on Molecular Dynamics and Enhanced Sampling Methods,

Institute for Computational Molecular Science, Temple University, USA.

Presentations

| 2017 | Talk: "Structure of APP-C99 1-99 and Implications for its Role |
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| | IN AMYLOIDOGENESIS," Kyoto University. |
| 2017 | POSTER: "ROLE OF CHOLESTEROL IN TERNARY LIPID MEMBRANE PHASE SE- |
| | PARATION OBSERVED VIA COARSE-GRAINED SIMULATIONS," American Theore- |
| | tical Chemistry Conference; Japanese Biophysical Society. |
| 2017 | POSTER: "TEMPERING IN OPENMM AND GENESIS," Temple Univerity; |
| | Current trends in molecular dynamics software design. |
| 2017 | TALK: "CRITICAL INVESTIGATION OF FINITE SIZE AND CHOLESTEROL EFFECTS |
| | IN LIPID DOMAIN FORMATION," RIKEN, Japan; Boston University Chemistry |
| | Graduate Student Seminar Series; Nagoya University IGER Seminar Series. |
| 2016 | POSTER: "EXPLORING PHASE SEPARATION AND DOMAIN FORMATION IN LIPID |
| | BILAYERS THROUGH MOLECULAR SIMULATION," Boston University Graduate |
| | Research Symposium; ACS 252nd National Meeting. |
| 2015 | Poster : "Examining the conformational dynamics of the N- |
| | TERMINAL REGION OF MDM2 USING MARKOV STATE MODEL APPROACHES," |
| | ACS 250th National Meeting. |
| 2015 | Talk: "Microsecond simulations of mdm2 and its complex with P53 |
| | YIELD INSIGHT INTO FORCE FIELD ACCURACY AND CONFORMATIONAL DYNA- |
| | MICS," Temple University Undergraduate Research Forum and Creative Works |
| | Symposium. |
| 2014-2015 | POSTER: "MICROSECOND SIMULATIONS OF MDM2 AND ITS COMPLEX WITH |
| | P53 YIELD INSIGHT INTO FORCE FIELD ACCURACY AND CONFORMATIONAL DY- |
| | NAMICS," ACS Philadelphia Younger Chemists Committee Conference; Emory |
| | STEM Research Symposium. |

Publications

- * \equiv Equal to first author contributions
- 11. "Aerosol-OT Surfactant Forms Stable Reverse Micelles in Aploar Solvent in the Absence of Water," R. Urano, G.A. Pantelopulos, J. E. Straub, Submitted (2018).
- 10. "Characterization of dynamics and mechanism in the self-assembly of AOT reverse micelles," R. Urano, G.A. Pantelopulos*, S. Song, J. E. Straub, Submitted (2018).
- 9. "Structural Role of Cholesterol in Complex Lipid Bilayer Phases Observed via MD Simulation," G.A. Pantelopulos, J. E. Straub Submitted (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* (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).