

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. <i>Boston University, USA.</i> Expected Graduation : 2019/5/19
2013-2015	B.S. OF CHEMISTRY. <i>Temple University, Philadelphia, USA.</i> Graduation : 2015/5/8
2011-2013	A.S. OF SCIENCE. <i>Community College of Philadelphia, Philadelphia, USA.</i> Graduation : 2013/5/4

Honors

2017	NSF GROW/JSPS FELLOW.
2015-Current	NSF GRADUATE RESEARCH FELLOWSHIP.
2015	PECO SCHOLAR.
2015	FEYNMAN MEMORIAL SCHOLAR.
2014-2015	UNDERGRADUATE RESEARCH FELLOW, <i>Temple University.</i>
2014	DIAMOND SCHOLAR SUMMER FELLOW, <i>Temple University.</i>
2013	HELLENIC UNIVERSITY CLUB SCHOLAR.
2013	NSF RESEARCH EXPERIENCE FOR UNDERGRADUATES, <i>Boston University.</i>
2013	AHEPA SCHOLAR.
2013	COMMUNITY COLLEGE OF PHILADELPHIA VOLUNTEER SERVICE AWARD.

Service

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.
2013	CHEMISTRY TUTOR, <i>Community College of Philadelphia.</i>

Extracurricular Training

2017	FRONTEIRS IN COMPUTATIONAL BIOPHYSICS AND BIOCHEMISTRY, <i>RIKEN, Japan.</i>
2016	ERICE SCHOOL : EXPLORING AND QUANTIFYING ROUGH FREE ENERGY LANDSCAPES, <i>International School of Statistical Physics, Ettore Majorana Foundation and Centre for Scientific Culture, Erice, Sicily, Italy.</i>
2015	ALAN ALDA COMMUNICATING SCIENCE WORKSHOP, <i>Boston University, USA.</i>
2015	SCHOOL ON MOLECULAR DYNAMICS AND ENHANCED SAMPLING METHODS, <i>Institute for Computational Molecular Science, Temple University, USA.</i>

Presentations

- 2017** POSTER : “TEMPERING IN OPENMM AND GENESIS,” *Temple University; 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 DYNAMICS,” *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 DYNAMICS,” *ACS Philadelphia Younger Chemists Committee Conference; Emory STEM Research Symposium.*
- 2013-2014** POSTER : “MOLECULAR DYNAMICS SIMULATIONS OF THE P53-MDM2 BINDING INTERFACE,” *ACS Philadelphia Younger Chemists Committee Conference; ACS 248th National Meeting.*

Publications

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).