

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 : 2019/5/19
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

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 HELLENIC UNIVERSITY CLUB SCHOLAR.
2013 NSF RESEARCH EXPERIENCE FOR UNDERGRADUATES, *Boston University.*
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, *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** 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.*
- 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. Accepted* (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. Accepted* (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).