

BRIGITA URBANC

CONTACT INFORMATION

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EDUCATION

- Ph.D., 1994 - Physics, Soft Condensed Matter; University of Ljubljana, Institute Jožef Stefan, Ljubljana, Slovenia. Thesis title: *Ferroelectric liquid crystals in external fields*.
- M.S., 1990 - Physics, University of Ljubljana, Institute Jožef Stefan, Ljubljana, Slovenia.
- B.S., 1987 - Physics, University of Ljubljana, Ljubljana, Slovenia.

ACADEMIC APPOINTMENTS

- Professor, Department of Biochemistry & Molecular Biology (secondary appointment), Drexel University College of Medicine, Philadelphia. 2019–present.
- Professor, Physics Department (primary appointment), Drexel University, Philadelphia. 2019–present.
- Associate Professor with Tenure, Physics Department, Drexel University, Philadelphia. 2014–2019.
- Docent za Fiziko, Fakulteta za Matematiko in Fiziko, University of Ljubljana, Slovenia. 2014–2019.
- Associate Professor, Physics Department, Drexel University, Philadelphia. 2008–present.
- Associate Research Professor, Physics Department, Boston University, Philadelphia. 2007–2008.
- Senior Research Associate, Boston University, Center for Polymer Studies, Boston. 2005–2007.
- Research Associate, Boston University, Center for Polymer Studies, Boston. 1999–2005.
- Visiting Scientist, Boston University, Center for Polymer Studies, Boston. 1994–1999.
- Research Associate, Theoretical Physics Department, Institute Jozef Stefan (IJS), Ljubljana (Slovenia). 1993–1999.

EXTRAMURAL FUNDING (As Independent Investigator)

09/01/2019–08/31/2023 (approved 1-year extension). **NSF OAC-1919691 Amendment ID 001** – MRI: *Proteus++: Enabling Data-Intensive Computing at Drexel University* PI: Gail Rosen (Electrical and Computer Engineering), Co-PIs: Hasan Ayaz (School of Biomedical Engineering, Science and Health Systems), **Brigita Urbanc** (Physics), Antonios Kontsos (Mechanical Engineering and Mechanics). Amendment Type: Supplement. Amendment Date: 07/13/2020. Amendment Number: 001. Proposal Number: 2039361. Amendment Description: Add supplemental support to the award NSF OAC-1919691. Amendment Award: \$24,000.

09/01/2019–08/31/2022. **NSF OAC-1919691** – MRI: *Proteus++: Enabling Data-Intensive Computing at Drexel University* PI: Gail Rosen (Electrical and Computer Engineering), Co-PIs: Hasan Ayaz (School of Biomedical Engineering, Science and Health Systems), **Brigita Urbanc** (Physics), Antonios Kontsos (Mechanical Engineering and Mechanics). Total Cost: \$542,740.

08/01/2018–07/31/2023 (approved 2nd-year extension). **NSF MCB-1817650** – *Moving toward an accurate molecular dynamics force field for intrinsically disordered proteins: Mission impossible?* PI: **Brigita Urbanc** (Drexel U, Physics); Co-PI: Reinhard Schweitzer-Stenner (Drexel U, Chemistry). Total Cost: \$554,614.

08/15/2017–07/31/2020. **NSF DMR-1707770** – *Identifying the rules governing tripeptide gelation in aqueous solution*. PI: Reinhard Schweitzer-Stenner (Drexel U, Chemistry); Co-PIs: Nicolas Alvarez (Drexel, Chem. & Biol. Engineering) and **Brigita Urbanc** (Drexel U, Physics). Total Cost: \$390,000.

- 08/15/2014–07/31/2017. **NSF DMR-1429661** – MRI: Development of a direct detection energy loss spectroscopy system. (PI: Mitra L. Taheri (Drexel U, Materials Science & Engineering); Co-PIs: Vibha Kalra (Drexel U, Chem. & Biol. Engineering), Steven J. May (Drexel U, Materials Science & Engineering), and **Brigita Urbanc** (Drexel U, Physics). Total Cost: \$870,676.
- 01/01/2015–12/31/2016. **Collaborative US-Slovenian Project** – MD simulations of the initial steps in oligomerization of an amyloidogenic protein human stefin B: Complex of stefin B oligomers with A β . PI: Eva Žerovnik (Institute Jozef Stefan, Biochem. & Mol. Biol., Slovenia), Co-PI: **Brigita Urbanc** (Drexel U, Physics). Total Cost: 3,570 EUR.
- 01/01/2012–12/31/2013. **Collaborative US-Slovenian Project** – MD simulations of the initial steps in oligomerization of an amyloidogenic protein human stefin B and comparison to the less amyloidogenic stefin A. PI: Eva Žerovnik (Institute Jozef Stefan, Biochem. & Mol. Biol., Slovenia), Co-PI: **Brigita Urbanc** (Drexel U, Physics). Total Cost: 3,920 EUR.
- 08/15/2008 - 07/31/2015. **NIH 2R01-AG021133** – Quantitative analysis of cerebral cortex in aging monkeys. PIs: H. Eugene Stanley (Boston U, Physics), Douglas Rosene (Boston U Medical School, Anatomy & Neurobiol.), and Luis Cruz (Drexel U, Physics). Total Cost: \$760,570 Role: Co-Investigator. Awarded \$84,089.
- 09/01/2008–07/31/2011. **NIH P01-AG027818** – Pathologic protein folding in human disease. Project 4: *Ab initio* molecular dynamics simulations of A β folding and assembly. PI: David B. Teplow (UCLA, Neurology), Project 4 Leader: H. Eugene Stanley (Boston U, Physics). Role: Co-Investigator and Drexel PI. Awarded \$568,294.

SUPERCOMPUTING RESOURCE ALLOCATION GRANTS

Access to the Extreme Science and Engineering Discovery Environment (XSEDE) facilities involves proposal applications, which are peer-reviewed. The awards are granted in Service Units (SU), where 1 SU corresponds to 1 CPU core/hr.

- 04/03/2019–04/02/2020. **MCB190028** – Self-assembly of GAG in Ethanol/Water Mixtures Examined by Molecular Dynamics. PI: **Brigita Urbanc**. Awarded: 1,600 Node Hours (estimated to \$415.36).
- 07/01/2010–09/30/2015. **PHY100030** – Multiscale molecular dynamics of protein folding and assembly. Full Allocation. PI: **Brigita Urbanc**. Awarded: 7,240,387 SUs.
- 07/01/2009–06/30/2010. **PHY100023** – Elucidation of the free energy folding landscapes of amyloid β -protein and α -synuclein, relevant to Alzheimer's and Parkinson's diseases. Startup Allocation. PI: **Brigita Urbanc**. Awarded: 500,000 SUs.
- 07/01/2009–06/30/2010. **MCB100030** – All-atom molecular dynamics simulations of amyloid β dimers. Startup Allocation. PI: Bogdan Barz (as a postdoctoral trainee in my group). Awarded: 500,000 SUs.

CONTRIBUTIONS TO EXTRAMURAL FUNDING (As Dependent Investigator)

- 08/01/2006–08/31/2008. **NIH P01-AG027818** – Pathologic protein folding in human disease. Project 4 *Ab initio* molecular dynamics simulations of A β folding and assembly. PI: David B. Teplow (UCLA, Neurology), Project 4 Leader: H. Eugene Stanley (Boston U, Physics). Role: Co-Investigator. Contribution: *de facto* Project 4 leader; spearheaded the application of discrete molecular dynamics to amyloid β -protein folding and aggregation and prepared the research proposal.
- 09/01/2005–05/31/2008. **NIH 1R01 AG021133** – Spatial analysis of cerebral cortex in aging monkeys. PI: H. Eugene Stanley (Boston U, Physics). Role: Research Associate. Contribution: preliminary research and grant preparation.
- 12/01/2005–11/30/2007. **Alzheimer's Association Zenith Fellowship** – Understanding formation of neurotoxic oligomers in Alzheimer's disease. PI: H. Eugene Stanley (Boston U, Physics). Role: Research Associate. Contribution: preliminary research and grant preparation.
- 12/01/2004–11/30/2006. **NIH R21 AG023661** – Molecular modeling of amyloid- β oligomer formation. PI: H. Eugene Stanley (Boston U, Physics). Role: Research Associate. Contribution: preliminary research and grant preparation.
- 07/01/2004–06/30/2006. **NIH R03 AG024633** – Methods for spatial analysis of microcolumns in cortex. PI: H. Eugene Stanley. Role: Research Associate. Contribution: grant application writing and preliminary research.

HONORS AND AWARDS

- Recognition by Drexel University Chapters of Sigma Pi Sigma and the Society of Physics Students for “her excellence in research and her support of the development of future scientists” (Drexel University, 03/02/2013).
- Drexel Travel Award to attend an invited talk at the International Meeting *Multiscale Modeling and Simulations of Hard and Soft Material* in Bangalore, India, 10/09/2009.
- Inclusion in the 60th Diamond Edition of MARQUIS Who’s Who in America, 2006–present.
- Bechtel Fellowship Award for the research on Alzheimer’s disease (Boston University, 2005–2007).
- Adler Foundation Fellowship for research on Alzheimer’s disease (Boston University, 1997–2000).
- Postdoctoral award from the Slovenian Ministry of Science (IJS, Ljubljana, 1993–1995).

PUBLICATIONS (in reverse chronological order)

Total Citations: **4,587**; h-Index: **34**; i10-Index: **58** (in *Google Scholar Citations*)

PEER REVIEWED PAPERS

79. B. Andrews, J. Guerra, R. Schweitzer-Stenner, **B. Urbanc**, *Do Molecular Dynamics Force Fields Accurately Model Ramachandran Distributions of Amino Acid Residues in Water?*, *Phys. Chem. Chem. Phys.* **24**, 3259-3279 (2022). [Times Cited:1]
78. B. Andrews, K. Long, and **B. Urbanc**, *Soluble State of Villin Headpiece Protein as a Tool in the Assessment of MD Force Fields*, *J. Phys. Chem. B*, Carol K. Hall Festschrift Virtual Special Issue, **125**, 6897-6911 (2021). [Times Cited:1]
77. **B. Urbanc**, *Cross-Linked Amyloid β -Protein Oligomers: A Missing Link in Alzheimer’s Disease Pathology?, invited perspective*, *J. Phys. Chem. B* **125**, 1307-1316 (2021). [Times Cited:4]
76. B. Milorey, R. Schweitzer-Stenner, B. Andrews, H. Schwalbe, and **B. Urbanc**, *Short peptides as predictors for the structure of polyarginine sequences in disordered proteins*, *Biophys. J.* **120**, 662-676 (2021). [Times Cited:8]
75. S. Zhang, B. Andrews, R. Schweitzer-Stenner, and **B. Urbanc**, *Intrinsic conformational dynamics of alanine in water/ethanol mixtures: An experiment-driven molecular dynamics study*, *J. Phys. Chem. B* **124**, 11600-11616 (2020). [Times Cited:5]
74. B. Andrews, S. Zhang, R. Schweitzer-Stenner, and **B. Urbanc**, *Glycine in Water Favors the Polyproline II State*, *Biomolecules* **10**, 1121 (2020). [Times Cited:9]
73. S. Zhang, R. Schweitzer-Stenner, and **B. Urbanc**, *Do molecular dynamics force fields capture conformational dynamics of alanine in water?*, *J. Chem. Theor. Comput.* **16**, 510-527 (2020); *J. Chem. Theor. Comput.* **16**, 5982 (2020). [Times Cited:17]
72. K. Long, T. L. Williams, **B. Urbanc**, *Insulin Inhibits A β 42 Aggregation and Prevents A β 42-Induced Membrane Disruption*, *Biochemistry* **58**, 4519-4529 (2019). [Times Cited:11]
71. S. Zhang, D. M. Fox, and **B. Urbanc**, *Elucidating the role of hydroxylated phenylalanine in formation and structure of cross-linked A β oligomers*, *J. Phys. Chem. B* **123**, 1068-1084 (2019). [Times Cited:7]
70. M. T. Mawhinney, R. Liu, F. Lu, J. Maksimoska, K. Damico, R. Marmorstein, P. M. Lieberman, and **B. Urbanc**, *CTCF-Induced Circular DNA Complexes Observed by Atomic Force Microscopy*, *J. Mol. Biol.* **430**, 759-776 (2018). [Times Cited:7]
69. M. T. Mawhinney, T. L. Williams, J. L. Hart, M. L. Taheri, and **B. Urbanc**, *Elucidation of Insulin Assembly in Acidic and Neutral pH: Characterization of Low Molecular Weight Oligomers*, *Proteins: Structure, Functions, and Bioinformatics* **85**, 2096-2110 (2017). [Times Cited:15]

68. M. J. Voelker, B. Barz, and **B. Urbanc**, Fully-Atomistic A β 40 and A β 42 Oligomers in Water: Observation of Pore-Like Conformations, *J. Chem. Theor. Comput.*, **13**, 4567-4583 (2017). Features cover art at <http://pubs.acs.org/toc/jctcce/13/9> [Times Cited:22]
67. S. Zhang, D. M. Fox and **B. Urbanc**, Insights Into Formation And Structure of A β Oligomers Cross-Linked Via Tyrosines, *J. Chem. Phys. B* **121**, 5523-5535 (2017). [Times Cited:17]
66. **B. Urbanc**, Flexible N-Termini of Amyloid β -Protein Oligomers: A Link between Structure and Activity?, in *Amyloid Aggregation*, Editors: Y. Miller and J. Straub, *Israel Journal of Chemistry* **57**, Special Issue 7-8, 651-664 (2017). [Times Cited:6]
65. M. Žganec, N. Kruczek, and **B. Urbanc**, Amino acid substitutions [K16A] and [K28A] distinctly affect amyloid β -protein oligomerization, *J. Biol. Phys.* **42**, 452-476 (2016). [Times Cited:11]
64. T.L. Williams, L.C. Serpell, and **B. Urbanc**, Stabilization of Native Amyloid β -Protein Oligomers by Copper and Hydrogen Peroxide Induced Cross-Linking of Unmodified Proteins (CHICUP), *Biochim. Biophys. Acta*, **1864**, 249-259 (2016). [Times Cited:34]
63. T.L. Williams, **B. Urbanc**, K.E. Marshall, D.M. Vadukul, A.T.A. Jenkins, and L.C. Serpell, Europium as an inhibitor of Amyloid- β (1-42) induced membrane permeation, *FEBS Lett.* **589**, 3228-3236 (2015). [Times Cited:10]
62. D. Meral, S. Toal, R. Schweitzer-Stenner, and **B. Urbanc**, Water-Centered Interpretation of Intrinsic pP Π Propensities of Amino Acid Residues: In Vitro-Driven Molecular Dynamics Study, *J. Phys. Chem. B* **119**, 13237-13251 (2015). [Times Cited:37]
61. D. Meral and **B. Urbanc**, Erratum to *Discrete Molecular Dynamics Study of Oligomer Formation by N-Terminally Truncated Amyloid β -Protein*, [*J. Mol. Biol.* **425**, 2260-2275 (2013)] *J. Mol. Biol.* **427**, 2726-2729 (2015). [Times Cited:7]
60. M. Žganec, E. Žerovnik, and **B. Urbanc**, Self-assembly of globular protein stefin B into polymorphic oligomers probed by discrete molecular dynamics, *J. Chem. Theor. Comput.* **11**, 2355-2366 (2015). [Times Cited:14]
59. M. Henderson, **B. Urbanc**, and L. Cruz, A Computational model for the loss of neuronal organization in microcolumns, *Biophys. J.* **106**, 2233-2242 (2014). [Times Cited:8]
58. B. Barz and **B. Urbanc**, Minimal model of self-assembly: Emergence of diversity and complexity, *J. Phys. Chem. B* **118**, 3761-3770 (2014). Features cover art at: http://pubs.acs.org/subscribe/covers/jpcbfbk/jpcbfbk_v118i014.jpg?0.3463436017051379 [Times Cited:27]
57. D. Meral and **B. Urbanc**, Discrete Molecular Dynamics Study of Oligomer Formation by N-Terminally Truncated Amyloid β -Protein, *J. Mol. Biol.* **425**, 2260-2275 (2013). [Times Cited:51]
56. S. Toal, D. Meral, D. Verbaro, **B. Urbanc**, and R. Schweitzer-Stenner, The pH-Independence of Trialanine and the Effects of Termini Blocking in Short Peptides: A Combined Vibrational, NMR, UVCD, and Molecular Dynamics Study, *J. Phys. Chem. B* **117**, 3689-3706 (2013). [Times Cited:66]
55. J.-E. Shea and **B. Urbanc**, Insights into A β aggregation: A molecular dynamics perspective, Special Issue: Protein Misfolding in Conformational Disorders, Guest Ed. Cláudio M. Gomes, *Curr. Top. Med. Chem.* **12**, 2596-2610 (2012). [Times Cited:53]
54. B. Barz, B.S. Turner, R. Bansil, and **B. Urbanc**, Folding of pig gastric mucin non-glycosylated domains: A discrete molecular dynamics study, *J. Biol. Phys.* **38**, 681-703 (2012). [Times Cited:21]
53. L. Cruz, J. S. Rao, D. B. Teplow, and **B. Urbanc**, Dynamics of Metastable β -Hairpin Structures in the Folding Nucleus of Amyloid β -Protein, *J. Phys. Chem. B* **116**, 6311-6325 (2012). [Times Cited:29]
52. B. Barz and **B. Urbanc**, Dimer Formation Enhances Structural Differences between Amyloid β -Protein (1-40) and (1-42): An Explicit-Solvent Molecular Dynamics Study, *PLoS One* **7**, e34345 (2012). [Times Cited:121]
51. A. Lam, D. B. Teplow, H. E. Stanley, and **B. Urbanc**, Erratum to *Effects of the Arctic mutation on the full length amyloid β -protein folding: A discrete molecular dynamics study* [*J. Am. Chem. Soc.* **130**, 17413-17422 (2008)] *J. Am. Chem. Soc.* **133**, 2789-2789 (2011). [Times Cited:2]

50. T. L. Williams, B. R. G. Johnson, **B. Urbanc**, A. T. A. Jenkins, S. D. A. Connell and L. C. Serpell, *Alzheimer's A β 42 oligomers, but not fibrils, simultaneously bind to and damage ganglioside containing lipid membranes*, *Biochem. J.* **439**, 67-77 (2011). [Times Cited:98]
49. **B. Urbanc**, M. Betnel, L. Cruz, H. Li, E. A. Fradinger, B. H. Monien, and G. Bitan, *Structural basis of A β ₁₋₄₂ toxicity inhibition by A β C-terminal fragments: Discrete molecular dynamics study*, *J. Mol. Biol.* **410**, 316-328 (2011). [Times Cited:55]
48. H. Li, B.H. Monien, A. Lomakin, R. Zemel1, E.A. Fradinger, M. Tan, S.M. Spring, **B. Urbanc**, C.-W. Xie, G.B. Benedek, and G. Bitan, *Mechanistic Investigation of the Inhibition of A β 42 Assembly and Neurotoxicity by C-terminal A β 42 Fragments*, *Biochemistry* **49**, 6358-6364 (2010). [Times Cited:59]
47. **B. Urbanc**, M. Betnel, L. Cruz, G. Bitan, and D.B. Teplow, *Elucidation of amyloid β -protein oligomerization mechanisms*, *J. Am. Chem. Soc.* **132**, 4266-4280 (2010). [Times Cited:252]
46. H. Li, B. H. Monien, E. A. Fradinger, **B. Urbanc**, and G. Bitan, *Biophysical Characterization of A β 42 C-terminal Fragments—Inhibitors of A β Assembly and Neurotoxicity*, *Biochemistry* **49**, 1259-1267 (2010). [Times Cited:55]
45. L. Cruz, D. L. Roe, **B. Urbanc**, A. Inglis, H. E. Stanley, and D. L. Rosene, *Age-related reduction in microcolumnar structure correlates with cognitive decline in ventral but not dorsal area 46 of the rhesus monkey*, *Neuroscience* **158**, 1509-1520 (2008). [Times Cited:33]
44. A. Lam, D. B. Teplow, H. E. Stanley, and **B. Urbanc**, *Effects of the Arctic mutation on the full length amyloid β -protein folding: A discrete molecular dynamics study*, *J. Am. Chem. Soc.* **130**, 17413-17422 (2008). [Times Cited:87]
43. E. Fradinger, B. H. Monien, **B. Urbanc**, A. Lomakin, M. Tan, H. Li, S. M. Spring, M. M. Condrón, L. Cruz, C.-W. Xie, G. B. Benedek and G. Bitan, *C-terminal peptides coassemble into A β 42 oligomers and protect neurons against A β 42-induced neurotoxicity*, *Proc. Natl. Acad. Sci. USA* **105**, 14175-14180 (2008). [Times Cited:198]
42. L. Cruz, **B. Urbanc**, A. Inglis; D. L. Rosene, and H. E. Stanley, *Generating a model of the three-dimensional spatial distribution of neurons using density maps*, *NeuroImage* **40**, 1105–1115 (2008). [Times Cited:19]
41. A. Inglis, L. Cruz, D. L. Roe, H. E. Stanley, D. L. Rosene, and **B. Urbanc**, *Automated identification of neurons and their locations*, *Journal of Microscopy* **230**, 339-347 (2008). [Times Cited:41]
40. S. Yun, **B. Urbanc**, L. Cruz, G. Bitan, D. B. Teplow, and H. E. Stanley, *Role of Electrostatic Interactions in Amyloid β -Protein Oligomer Formation: A Discrete Molecular Dynamics Study*, *Biophys. J.* **92**, 4064–4077 (2007). [Times Cited:154]
39. D. B. Teplow, N. D. Lazo, G. Bitan, S. Bernstein, T. Wyttenbach, M. T. Bowers, A. Baumketner, J.-E. Shea, **B. Urbanc**, L. Cruz, J. Borreguero, and H. E. Stanley, *Elucidating Amyloid β -Protein Folding and Assembly: A Multidisciplinary Approach*, *Account of Chemical Research* **39**, 635–645 (2006). [Times Cited:253]
38. **B. Urbanc**, L. Cruz, D. B. Teplow, and H. E. Stanley, *Computer Simulations of Alzheimer's Amyloid β -Protein Folding and Assembly*, *Current Alzheimer Research* **3**, 493–504 (2006). [Times Cited:67]
37. L. Cruz, **B. Urbanc**, J. M. Borreguero, N. D. Lazo, D. B. Teplow, and H. E. Stanley, *Solvent and mutation effects on the nucleation of amyloid β -protein folding*, *Proc. Natl. Acad. Sci. USA* **102**, 18258–18263 (2005). [Times Cited:141]
36. J. M. Borreguero, **B. Urbanc**, N. D. Lazo, S. V. Buldyrev, D. B. Teplow, and H. E. Stanley, *Folding events in the 21-30 region of amyloid β -protein (A β) studied in silico*, *Proc. Natl. Acad. Sci. USA* **102**, 6015–6020 (2005). [Times Cited:149]
35. L. Cruz, S. V. Buldyrev, S. Peng, D. L. Roe, **B. Urbanc**, H. E. Stanley, and D. L. Rosene, *A statistically based density map method for identification and quantification of regional differences in microcolumnarity in the monkey brain*, *J. Neurosci. Methods* **141**, 321–332 (2005). [Times Cited:39]
34. **B. Urbanc**, L. Cruz, S. Yun, S. V. Buldyrev, G. Bitan, D. B. Teplow, and H. E. Stanley, *In silico study of amyloid β -protein folding and oligomerization*, *Proc. Natl. Acad. Sci. USA* **101**, 17345–17350 (2004). [Times Cited:399]

33. L. Cruz, D. L. Roe, **B. Urbanc**, H. Cabral, H. E. Stanley, and D. L. Rosene, *Age-related reduction in microcolumnar structure in area 46 of the rhesus monkey correlates with behavioral decline*, *Proc. Natl. Acad. Sci. USA* **101**, 15846–15851 (2004). [Times Cited:46]
32. **B. Urbanc**, L. Cruz, F. Ding, D. Sammond, S. Khare, S. V. Buldyrev, H. E. Stanley, and N. V. Dokholyan, *Molecular Dynamics Simulation of Amyloid β Dimer Formation*, *Biophys. J.* **87**, 2310–2321 (2004). [Times Cited:241]
31. S. Peng, F. Ding, **B. Urbanc**, S. V. Buldyrev, L. Cruz, H. E. Stanley, and N. V. Dokholyan, *Discrete molecular dynamics simulations of peptide aggregation*, *Phys. Rev. E* **69**, 041908 (2004). [Times Cited:105]
30. S. Peng, **B. Urbanc**, L. Cruz, B. T. Hyman, and H. E. Stanley, *Neuron recognition by parallel Potts segmentation*, *Proc. Natl. Acad. Sci. USA* **100**, 3847–3852 (2003). [Times Cited:29]
29. **B. Urbanc**, L. Cruz, R. Le, J. Sanders, K. Hsiao-Ashe, K. Duff, H. E. Stanley, M. C. Irizarry and B. T. Hyman, *Neurotoxic effects of thioflavin S-positive amyloid deposits in transgenic mice and Alzheimer's disease*, *Proc. Natl. Acad. Sci. USA* **99**, 13990–13995 (2002). [Times Cited:257]
28. R. Le, L. Cruz, **B. Urbanc**, R. B. Knowles, K. Hsiao-Ashe, K. Duff, M. Irizarry H. E. Stanley, and B. T. Hyman, *Plaque-Induced Abnormalities in Neurite Geometry in Transgenic Models of Alzheimer's Disease: Implications for Neural System Disruption*, *J. Neuropath. Exp. Neurol.* **60**, 763–758 (2001). [Times Cited:106]
27. S. V. Buldyrev, L. Cruz, T. Gomez-Isla, E. Gomez-Tortosa, S. Havlin, R. Le, H. E. Stanley, **B. Urbanc** and B. T. Hyman, *Description of microcolumnar ensembles in association cortex and their disruption in Alzheimer and Lewy body dementias*, *Proc. Natl. Acad. Sci. USA* **97**, 5039–5043 (2000). [Times Cited:116]
26. R. B. Knowles, C. Wyart, S. V. Buldyrev, L. Cruz, **B. Urbanc**, M. E. Hasselmo, H. E. Stanley, and B. T. Hyman, *Plaque-induced neurite abnormalities: Implications for disruption of neural networks in Alzheimer's disease*, *Proc. Natl. Acad. Sci. USA* **96**, 5274–5279 (1999). [Times Cited:296]
25. **B. Urbanc**, L. Cruz, S. V. Buldyrev, S. Havlin, B. T. Hyman, and H. E. Stanley, *Dynamic feedback in an aggregation–disaggregation model*, *Phys. Rev. E* **60**, 2120–2126 (1999). [Times Cited:25]
24. **B. Urbanc**, L. Cruz, S. V. Buldyrev, S. Havlin, M. C. Irizarry, H. E. Stanley, and B. T. Hyman, *Dynamics of Plaque Formation in Alzheimer's Disease*, *Biophys. J.* **76**, 1330–1334, (1999). [Times Cited:84]
23. H. E. Stanley, S. V. Buldyrev, L. Cruz, T. Gomez-Isla, S. Havlin, B. T. Hyman, R. Knowles, **B. Urbanc** and C. Wyart, *Statistical Physics and Alzheimer's Disease* [Proc. Bar-Ilan Conf], *Physica A* **249**, 460–471 (1998). [Times Cited:22]
22. **B. Urbanc** and L. Cruz, *Order parameter and segregated phases in a sandpile model with two particle sizes*, *Phys. Rev. E* **56**, 1571–1579 (1997). [Times Cited:6]
21. L. Cruz, **B. Urbanc**, S. V. Buldyrev, R. Christie, T. Gómez-Isla, S. Havlin, M. McNamara, H. E. Stanley, and B. T. Hyman, *Aggregation and disaggregation of senile plaques in Alzheimer disease*, *Proc. Natl. Acad. Sci. USA* **94**, 7612–7616 (1997). [Times Cited:128]
20. **B. Kutnjak-Urbanc**, S. Havlin, H. E. Stanley, *Temporal correlations in a one-dimensional sandpile model*, *Phys. Rev. E* **54**, 6109–6113 (1996). [Times Cited:13]
19. **B. Kutnjak-Urbanc**, S. Zapperi, S. Milošević, H. E. Stanley, *Sandpile model on the Sierpinski gasket fractal*, *Phys. Rev. E* **54**, 272–277 (1996). [Times Cited:43]
18. **B. Kutnjak-Urbanc**, B. Žekš, *Phase excitation spectrum of ferroelectric liquid crystals in an external static electric field*, *Phys. Rev. E* **52**, 3892–3903 (1995). [Times Cited:15]
17. **B. Kutnjak-Urbanc**, B. Žekš, *Behavior of ferroelectric liquid crystals in external fields*, *Phys. Rev. E* **51**, 1569–1572 (1995). [Times Cited:14]
16. **B. Kutnjak-Urbanc**, B. Žekš, *Microscopic origin of spontaneous polarization in ferroelectric SmC* liquid crystals*, *Liq. Cryst.* **18**, 483–488 (1995). [Times Cited:17]
15. B. Žekš, T. Carlsson, I. Mušević, **B. Kutnjak-Urbanc**, *Dielectric response of ferroelectric liquid crystals in bias electric field*, *Liq. Cryst.* **15**, 103–111 (1993). [Times Cited:14]

14. **B. Kutnjak-Urbanc**, B. Žekš, B. Rovšek, *The influence of finite dimensions on the static ordering of the SmC* phase in an electric field*, *Liq. Cryst.* **14**, 999–1005 (1993). [Times Cited:3]
13. **B. Kutnjak-Urbanc**, B. Žekš, *Theoretical investigation of the behavior of ferroelectric liquid crystals in a magnetic or in a high-frequency electric field*, *Phys. Rev. E* **48**, 455–464 (1993). [Times Cited:18]
12. B. Žekš, **B. Urbanc**, *The microscopic model of polar and quadrupolar ordering in ferroelectric smectic C* liquid crystals*, *Ferroelectrics* **113**, 151–162 (1991). [Times Cited:8]
11. **B. Urbanc**, B. Žekš, T. Carlsson, *Nonlinear effects in the dielectric response of ferroelectric liquid crystals*, *Ferroelectrics* **113**, 219–230 (1991). [Times Cited:24]
10. **B. Urbanc**, B. Žekš, *Microscopic model of the spontaneous polarization in ferroelectric liquid crystals*, *Liq. Cryst.* **5**, 1075–1082 (1989). [Times Cited:52]
9. B. Žekš, T. Carlsson, C. Filipič, **B. Urbanc**, *Thermodynamic model of ferroelectric liquid crystals and its microscopic basis*, *Ferroelectrics* **84**, 3–14 (1988). [Times Cited:65]

INVITED BOOK CHAPTERS (with Editorial Review)

8. **B. Urbanc**, *Perplexity of Amyloid β -Protein Oligomer Formation: Relevance to Alzheimer's Disease*, Ch.1 in *Biophysics and Biochemistry of Protein Folding and Aggregation*, Eds. J.-M. Yuan and H.-X. Zhou, World Scientific, Co., Singapore, Vol. 9, 1-50 (2017). Features Cover Art. [Times Cited:2]
7. A. Attar, D. Meral, **B. Urbanc**, and G. Bitan, *Assembly of Amyloid β -Protein Variants Containing Familial Alzheimer's Disease-Linked Amino Acid Substitutions*, Chapter 38 in *Bio-nanoimaging: Protein Misfolding and Aggregation*, Eds. V. Uversky and Y. Lyubchenko, Elsevier, Pages 429-442 (2014). [Times Cited:10]
6. M. Betnel, N.V. Dokholyan, and **B. Urbanc**, *From disordered amyloid β -proteins to soluble oligomers and protofibrils using Discrete Molecular Dynamics*, in *Alzheimer's disease: Molecular basis of amyloid- β protein aggregation and fibril formation—Insights into low molecular weight and cytotoxic aggregates from computer simulations*, *Molecular Medicine and Medicinal Chemistry* **7**, Part B, Ch. 12, 333-358, Ed. P. Derreumaux, Imperial College Press (2013). [Times Cited:2]
5. J. Srinivasa Rao, **B. Urbanc**, and L. Cruz, *Ch.16: Computational studies of folding and assembly of amyloidogenic proteins*, in *Folding, Misfolding and Nonfolding of Peptides and Small Proteins*, Ed. R. Schweitzer-Stenner, John Wiley & Sons, Inc., Hoboken, NJ, USA; 479-527, (2012).
4. **B. Urbanc**, J.M. Borreguero, L. Cruz, and H.E. Stanley, *Ab initio discrete molecular dynamics approach to protein folding and aggregation*, *Methods in Enzymology* **412**, Ch.19, 314–338 (2006). [Times Cited:81]

PROCEEDINGS PAPERS (with Editorial Review)

3. A. Lam, **B. Urbanc**, J. M. Borreguero, N. D. Lazo, D. B. Teplow, and H. E. Stanley, *Discrete Molecular Dynamics Study of Alzheimer Amyloid β -protein ($A\beta$) Folding*, *Proceedings of The 2006 International Conference on Bioinformatics & Computational Biology*, CSREA Press, Las Vegas, Nevada, 322–328 (2006). [Times Cited:9]
2. **B. Urbanc** and M. Čepič, *Possible Isostructural Transitions in the Ferroelectric Liquid Crystals in High External Electric Fields*, [20th International Liquid Crystal Conference, 2004, Ljubljana (Slovenia)] *Mol. Cryst. Liq. Cryst.* **438**, 41(1605)–46(1610) (2005).
1. **B. Kutnjak-Urbanc**, B. Žekš, in *Phase transitions in Liquid Crystals*, Edited by S. Martellucci and A. N. Chester, *The phase transition from the SmC* to the SmC phase induced by an external magnetic field*, Ch.23, Plenum, New York (1992). [Times Cited:5]

PRESENTATIONS (in reverse chronological order)

INVITED TALKS

116. *Amyloid β -protein folding and oligomer formation: Molecular dynamics perspective*, Department of Physics, New Jersey Institute of Technology, invited seminar, 19 September, 2022.
115. *Current issues with molecular dynamics force fields for intrinsically disordered proteins*, Biological Physics & Physical Biology Seminar Series (<https://sites.google.com/view/bppb-seminar/bppb-seminar-2022>), 26 August, 2022.
114. *Biophysical insights into amyloid β -protein oligomer formation*, invited seminar at the Gustaf H. Carlson School of Chemistry and Biochemistry, Clark University, 22 April, 2022.
113. *Do MD simulations capture intrinsic conformational propensities of amino acid residues in water?*, invited talk at the 17th Theoretical Chemistry Symposium (TCS2021), Indian Institute of Science Education and Research (IISER), Kolkata, India, 11-14 December, 2021.
112. *Biophysics of Amyloid β -Protein Oligomer Formation of Relevance to Alzheimer's Disease*, *Journal of Biological Physics* Webinar Series (remote synchronous), 18 May 2021.
111. *Dichotomy of Amyloid β -Protein Assembly in Alzheimer's Disease*, Seminar (remote synchronous), Biophysical Society (Društvo Biofizikov) University in Ljubljana, Slovenia, 13 May 2021.
110. *Conformational Dynamics of Short Peptides in Aqueous Solutions: Assessment of Molecular Dynamics Force Fields*, Annual Meeting of the Mid Atlantic Section of the American Physical Society (MAS-APS), Session *Protein and Lipid Dynamics*, & Chair of the Session on *Biomolecular Assemblies*, 6 December 2020 (remote synchronous).
109. *Biophysics of Intrinsically Disordered Proteins*, invited seminar in the Department of Biochemistry and Molecular Biology at Drexel Medical School, 31 August 2020 (remote synchronous).
108. *Do MD Force Fields Capture Conformational Dynamics of Amino Acid Residues in Water?*, Gordon Research Conference on *Protein Folding Dynamics*, 5-10 January 2020, Galveston, Texas.
107. *Biophysics of Protein Assembly and Its Relevance to Human Disease*, World Congress of Slovenian Physicists (translated from *Svetovni kongres slovenskih fizikov*), 4-5 July 2019, Ljubljana (Slovenia).
106. *Insights into Cross-Linked Amyloid β -Protein Oligomers and Their Role in Alzheimer's Disease*, Protein Aggregation, N1.00005, APS Mid-Atlantic Section Meeting, 3-5 November 2017, Newark, NJ.
105. *Computational and Experimental Findings on Protein Self-Assembly and Its Relevance to Human Disease*, Colloquium, Villanova University, Department of Physics, 29 September 2017, Villanova, PA.
104. *Amyloid Protein Self-Assembly Examined Through Computer Simulations*, Bio Big Data Journal Club, hosted by *College of Computing & Informatics*, Drexel University, 4 June 2015, Philadelphia, PA 19104.
103. *Perplexity of Amyloid Protein Assembly Examined Through In Vitro-Driven Discrete Molecular Dynamics*, Philadelphia Theoretical Chemistry Club, organized by Joshua Schrier (Haverford), Joseph Subotnik (Penn), Michelle Francl (Bryn Mawr), and Paul Rablen (Swarthmore) and funded by the Mellon Foundation, Inaugural Talk, Bryn Mawr College, 6 May 2015, PA.
102. *Perplexity of Amyloid Protein Self-Assembly: A Minimalist View*, Physics Seminar, Widener University. 1 December 2014, Chester, PA 19013.
101. *Amyloid β -Protein Assembly in the Presence of Inert Crowders*, Telluride workshop, entitled "Protein and Peptide Interactions in Cellular Environments", 23-27 June 2014, Telluride, CO.
100. *Elucidating Specificity and Universality of Amyloid Protein Self-Assembly*, Department of Physics, University of Ljubljana, 2 May 2014, Slovenia.
99. *Insights into specificity and universality of protein self-assembly*, Physics Colloquium, Drexel University, 24 October 2013, Philadelphia.

98. *Insights into amyloid β -protein self-assembly: Specificity versus universality*, Biophysics Seminar, Boston University, 18 October 2013, Boston.
97. *The Role of Physics in Understanding And Tackling Alzheimer's Disease*, Keynote Speaker, Sigma Pi Sigma Induction Ceremony, Drexel Chapter, Drexel University, 2 March 2013, Philadelphia.
96. *Elucidation of amyloid β -protein assembly and toxicity inhibition*, Institute Jožef Stefan, Department of Biochemistry, Molecular and Structural Biology, 28 May 2012, Ljubljana, Slovenia.
95. *Elucidation of amyloid β -protein oligomer formation in the absence and presence of toxicity inhibitors*, CECAM Workshop on *Anchoring simulations to experiments: challenges for understanding and treating Alzheimer's disease*, 21-23 May 2012, Paris, France.
94. *Biophysics of amyloid β -protein folding and assembly: Relevance to Alzheimer's disease*, Colloquium, Department of Physics, University of Missouri at St. Louis, 13 April 2012, St. Louis.
93. *Unraveling Diseases Associated with Aberrant Protein Assembly: A Physicist's Approach*, Talk for Society for Physics Students at Drexel University, 14 May 2010.
92. *Discrete molecular dynamics simulations of amyloid β -protein assembly*, Talk at the conference "Multiscale Modeling and Simulations of Hard and Soft Materials," Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore, India, 19 December 2009.
91. *Computational studies of amyloid β -protein assembly relevant to Alzheimer's disease*, Colloquium, University of Delaware, Physics Department, Newark, 7 October 2009.
90. *Protein structure-toxicity relationship relevant to Alzheimer's disease: Discrete molecular dynamics study*, Session "Molecular Basis of Protein Aggregation and Amyloid Formation," 2009 Fall American Chemical Society Meeting, Washington DC, ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY **238**, Meeting Abstract: **229-PHYS**, 2009.
89. *The Role of Computer Simulations in Therapeutic Approaches to Alzheimer's Disease*, Yeshiva University, New York City, 12 May 2009.
88. *The Role of Computer Simulation in Therapeutic Approaches to Alzheimer's Disease*, Dean's Seminar Series, Drexel University, Philadelphia, 19 November 2008.
87. *Amyloid β -Protein Folding and Assembly: Ab Initio Discrete Molecular Dynamics Approach*, UCLA, David Geffen School of Medicine, Department of Neuroscience, Los Angeles, 29 April 2008.
86. *Alzheimer's Amyloid β -Protein Folding and Assembly: Discrete Molecular Dynamics Approach*, Drexel University, Physics Department, Philadelphia, 13 March 2008.
85. *Ab Initio Discrete Molecular Dynamics Approach to Studies of Alzheimer's Amyloid β -Protein Folding and Assembly*, Biophysics Seminar, Boston University, Physics Department, Boston, 16 Nov. 2007.
84. *Amyloid β -Protein Assembly in the Presence of Peptide Inhibitors*, The 2007 NCTS October Workshop on Critical Phenomena and Complex Systems, Taipei, 15 October 2007.
83. *Oligomer Formation of Alzheimer's Amyloid β -Proteins A β 40 and A β 42*, The 2007 NCTS October Workshop on Critical Phenomena and Complex Systems, Taipei, 13 October 2007.
82. *Ab Initio Discrete Molecular Dynamics Approach to Studies of Protein Folding and Assembly*, The 2007 NCTS October Workshop on Critical Phenomena and Complex Systems, Taipei, 12 October 2007.
81. *In vitro driven computer simulations of relevance to Alzheimer's disease*, Biophysical Society Meeting, Baltimore, March 2007.
80. *In vitro driven computer simulations of relevance to Alzheimer's disease*, Society for Neuroscience 2006: Satellite Symposium, Atlanta, October 2006.
79. *Statistical Physics Approach to Understanding Alzheimer's Disease*, California State University at Northridge, Physics Department, Los Angeles, 12 Dec. 2005.

78. *In silico study of amyloid- β folding and oligomer formation*, American Chemical Society Meeting, San Diego, 2005.
77. *Molecular Dynamics Simulation of Amyloid- β Dimer Formation*, Second ICAM Workshop on Physical Principles of Amyloid Diseases: "Protein Misaggregation: From Molecules To Neurodegeneration," Boston, 2004.
76. *Microscopic model for spontaneous polarization in ferroelectric liquid crystals*, University of Puerto Rico, Rio Piedras, San Juan, 1997.

OUTREACH TALKS

75. *Molecular Biophysics of Protein Assembly and Its Relevance to Human Disease*, Invited Talk and Panel Discussion, *PA Young Women in Physics* Conference, Bucknell University, PA, 7 April 2018.
74. *Physics and Alzheimer's Disease*, Invited Informal Talk and Discussion with high school students working on *Ice Cube* project, organized by Naoko Kurahashi Nielson and Christina Love, 24 August 2016; 7 July 2017.
73. *Physics of Intrinsically Disordered Students ... OOPS Proteins, not Students*, Kaczmarczik Day, Drexel University, Philadelphia, 9 February 2016.
72. Invited 40-minute workshop on *Protein Folding* at the CATALYST conference for middle school female students interested in natural sciences, Swarthmore College, Swarthmore, PA, 17 March 2012.
71. *My Physics Career Pathway: A Curiosity-Driven Ride*, Invited Talk, Women in Physics Society (WIPS) 2 December 2011, Drexel University.
70. *Curiosity-driven ride through uncertainties of my physics career pathway*, Invited Talk, Boston University, *Women in Physics*, Boston, 28 May 2008.

ORAL AND POSTER PRESENTATIONS

69. **B. Andrews**, S. Zhang, R. Schweitzer-Stenner, and B. Urbanc, *Assessing the Ability of Molecular Dynamics Force Fields to Capture Conformational Dynamics of Amino Acid Residues in Water*, Bulletin of the American Physical Society, 2022 APS March Meeting, contributed talk, meeting abstract F06. 00002 (2022).
68. **B. Andrews**, S. Zhang, R. Schweitzer-Stenner, and B. Urbanc, *Glycine Shows Preference for Polyproline II Indicating Greater Role for Amino Acid Backbone*, Bulletin of the American Physical Society, 2021 APS March Meeting, contributed talk, meeting abstract P12.00005 (2021).
67. **B. Milorey**, R. Schweitzer-Stenner, B. Andrews, H. Schwalbe, and B. Urbanc, *Short arginine-based peptides as predictors for the extended structure of polyarginine sequences in intrinsically disordered proteins*, Biophys. J. **120**, 99A-100A, Supplement 1, meeting abstract, contributed talk 479-Plat (2021).
66. **S. Zhang**, B. Andrews, R. Schweitzer-Stenner, and B. Urbanc, *An Experiment-Driven Molecular Dynamics Study of GAG in Water/Ethanol Mixtures*, Mid-Atlantic Section Fall Meeting 2020, Session K01: Protein and Lipid Dynamics, contributed talk K01.00004, Volume **65**, Number 20, December 4-6 (2020).
65. **B. Andrews**, K. Long, and B. Urbanc, *Examining the Self Assembly of the Villin Headpiece Protein: A Combined Experimental and Molecular Dynamics Study** Mid-Atlantic Section Fall Meeting 2020, Session K01: Protein and Lipid Dynamics, contributed talk K01.00005, Volume **65**, Number 20, December 4-6 (2020).
64. S. Zhang, R. Schweitzer-Stenner, B. Urbanc, *The Assessment of MD Force Fields with Respect to Alanine Conformations in Aqueous Solutions*, Bulletin of the American Physical Society **65**, contributed talk D22.00007 (2020).
63. S. Zhang, R. Schweitzer-Stenner, and B. Urbanc, *Conformational Dynamics of Alanine in Water and Water/Ethanol Mixtures: Experimentally Driven Evaluation of Molecular Dynamics Force Field*, Biophys. J. **118**, 502A-502A, meeting abstract: 2455-Pos (2020).

62. K. Long, T. L. Williams, and B. Urbanc, *In Vitro Study of the Effect of Insulin on Amyloid β -Protein Assembly and Toxicity*, 63th Annual Meeting of Biophysical Society (Baltimore, 2-6 March 2019), *Biophys. J.* **116**, 458A-458A, Meeting Abstract: 2267-Plat (2019).
61. S. Zhang, C. Trinh, R. Schweitzer-Stenner, and B. Urbanc, *Self-Assembly of GAG in Ethanol/Water Mixtures Examined by Molecular Dynamics*, 63th Annual Meeting of Biophysical Society (Baltimore, 2-6 March 2019), *Biophys. J.* **116**, 61A-61A, Meeting Abstract: 308-Pos (2019).
60. K. Long, T. L. Williams, and B. Urbanc *Insulin assembly at neutral pH: Comparison and relevance to $A\beta$ assembly*, poster presentation (MAS17-2017-000290), Mid-Atlantic Section meeting of APS, 3-5 November 2017, Newark, NJ.
59. S. Zhang, D. M. Fox, and B. Urbanc, *Insights into the effect of cross-linking on $A\beta$ oligomer formation and structure*, poster presentation (MAS17-2017-000291), Mid-Atlantic Section meeting of APS, 3-5 November 2017, Newark, NJ.
58. B. Antos and B. Urbanc, *A Coarse-grained lipid bilayer model for studies of amyloid β -protein–membrane interactions* oral presentation, Drexel University Research Day, April 27, 2017.
57. S. Zhang, D. M. Fox, and B. Urbanc, *Insights Into Formation And Structure Of $A\beta$ Oligomers Cross-Linked Via Tyrosines*, poster presentation, Drexel University Research Day, 27 April 2017.
56. M. T. Mawhinney, T. L. Williams, and B. Urbanc, *Elucidation of insulin assembly pathways using biophysical methods* invited seminar, Department of Physics, Saint Joseph's University, Philadelphia PA, 30 Mar 2016.
55. M. J. Voelker and B. Urbanc, *A Computational Study of Amyloid β -Protein Assembly in Crowded Environments*, poster presentation, *Biophys. J.* **108**, (2), S1 (525A-525A), Meeting Abstract: 2656-Pos, 27 Jan. 2015.
54. D. Meral and B. Urbanc, *DMD4B-HYDRA: Toward a Novel Discrete Molecular Dynamics Protein Model*, poster presentation, *Biophys. J.* **108**, (2), S1 (157A-157A), Meeting Abstract: 783-Pos, 27 Jan. 2015.
53. M. T. Mawhinney, T. L. Williams, and B. Urbanc, *Elucidating the role of oligomers in insulin aggregation using biophysical methods*, poster presentation, Biophysical Society 59th Annual Meeting, Baltimore MD, 10 Feb. 2015.
52. M. Žganec, E. Žerovnik, and B. Urbanc, *DMD simulations of folding and early stages of oligomerization of stefins*, poster presentation, Regional Biophysics Conference Smolenice, Slovakia 2014-05-15–2014-05-20.
51. A. Tomida, D. Meral, and B. Urbanc, *The Effect of Amino Acid Substitutions at Position 2 on $A\beta$ Folding and Oligomer Formation*, poster presentation, Research Day, College of Arts and Sciences, Drexel University, March 2014.
50. M. T. Mawhinney, T. L. Williams, and B. Urbanc, *Elucidating the role of tetramers on insulin aggregation using biophysical methods*, poster presentation, Research Day, College of Arts and Sciences, Drexel University, March 2014.
49. M. J. Voelker, M. Betnel, and B. Urbanc, *A Discrete Molecular Dynamics Study of α -Synuclein Folding and Oligomer Assembly*, poster presentation, Research Day, College of Arts and Sciences, Drexel University, March 2014.
48. D. Meral and B. Urbanc, *ProtsDMD: Toward a Novel Discrete Molecular Dynamics Protein Model*, poster presentation, Research Day, College of Arts and Sciences, Drexel University, March 2014.
47. M. Žganec, E. Žerovnik, and B. Urbanc, *Folding and early stages of oligomerization of stefins*, oral presentation, Dneva biofizike, Rogla, Slovenia, 2013-11-28–2013-11-29.
46. W. Morrison, E. L. Giannaris, L. Cruz, F. Mortazavi, B. Urbanc, J. Santos, D. L. Rosene, and H. E. Stanley, *Microcolumnar properties show sexual dimorphism in areas 17 and 46 of monkey brain*, poster presentation, The Annual Society for Neuroscience Meeting, San Diego, November 2013.
45. G.B. Benedek, H. Li, B. H. Monien, A. Lomakin, R. Zemel, E. A. Fradinger, M. Tan, S. M. Spring, B. Urbanc, C.-W. Xie, and G. Bitan, *Mechanistic Investigation of the Inhibition of $A\beta_{42}$ Assembly and Neurotoxicity by $A\beta_{42}$ C-terminal Fragments*, oral presentation, American Chemical Society (ACS) Meeting Abstracts, 2013.
44. T. L. Williams and B. Urbanc, *Addition of Sugars to Alzheimers $A\beta$ Peptide Significantly Affects Oligomeric Distribution of the Peptide and Permeation of Biomimetic Lipid Vesicles*, poster presentation, at the meeting on *Translating Natural Products into Drugs for Alzheimer's and Neurodegenerative Disease*, The New York Academy of Sciences, New York City, 6 May 2013.

43. D. Meral and B. Urbanc, *Discrete Molecular Dynamics Study of Oligomer Formation by N-Terminally Truncated Amyloid β -Protein*, poster presentation, The Biophysical Society Meeting, Philadelphia, *Biophys. J.* **104**, 389A-389A (2013).
42. D. M. Fox, B. Barz, and B. Urbanc, *The Role of Di-Tyrosine Bonding in Amyloid β -Assembly*, poster presentation, The Biophysical Society Meeting, Philadelphia, *Biophys. J.* **104**, 391A-391A (2013).
41. M. Žganec, E. Žerovnik, B. Urbanc, *DMD simulations of stefin folding and early stages of oligomerization*, oral presentation, 11th Greta Pifat-Mrzljak International School of Biophysics Primošten, Croatia, 2012-09-30 - 2012-10-09.
40. T. L. Williams, D. M. Fox, B. Barz, M. M. Condrón, D.B. Teplow, and B. Urbanc, *N-Terminal Modification Results in More Compact Amyloid β -Protein Oligomers with a Reduced Ability to Cause Membrane Permeation*, poster presentation, The Annual Society for Neuroscience Meeting, New Orleans, October 2012.
39. T. L. Williams and B. Urbanc, *Addition of Sugars to Alzheimer's A β Peptide Significantly Affects Oligomeric Distribution of the Peptide and Permeation of Biomimetic Lipid Vesicles*, poster presentation, University Research Day, Drexel University, April 2012.
38. R. Liu, G. Yang, P. Lieberman, and B. Urbanc, *Investigation of the interaction between CTCF and DNA using AFM imaging*, poster presentation, CoAS Research Day, Drexel University, 2012 (the poster won 3rd place in Graduate Sciences category).
37. D. Meral and B. Urbanc, *Early Assembly Events of N-terminally Truncated Form of Amyloid β -Protein*, poster presentation, University Research Day, Drexel University, April 2012.
36. D. Meral and B. Urbanc, *Early Assembly Events of N-terminally Truncated Form of Amyloid β -Protein*, poster presentation, CoAS Research Day, Drexel University, April 2012 (the poster won 1st place in Graduate Sciences category).
35. D. Verbaro, D. Meral, B. Urbanc, K. Rybka, H. Schwalbe, R. Schweitzer-Stenner, *Is the Amino Acid Dipeptide a Suitable Model for Investigating Structural Preferences in the Unfolded State?*, poster presentation, *Biophys. J.* **102**, 253A-253A (2012).
34. P. Massey, B. Barz, and B. Urbanc, *Structural elements involved in mediating amyloid β -protein toxicity in Alzheimer's disease*, poster presentation, Neuroscience 2011, Society for Neuroscience, Washington DC, November 2011.
33. D. Meral and B. Urbanc, *Early assembly events of N-terminally truncated forms of amyloid β -protein*, oral presentation, Neuroscience 2011, Society for Neuroscience, Washington DC, November 2011.
32. B. Barz and B. Urbanc, *All-atom molecular dynamics stability study of amyloid β -protein (1-40) and (1-42) oligomers relevant to Alzheimer's disease*, oral presentation, Neuroscience 2011, Society for Neuroscience, Washington DC, November 2011.
31. B. Barz, C. Kepics, F. Ferrone, and B. Urbanc, *Minimalistic approach to protein assembly modeling / Application to the sickle cell hemoglobin polymerization*, poster presentation, Biophysical Society 55th Annual Meeting, Baltimore, *Biophys. J.* **100**, 389-389 (2011).
30. B. Barz, C. Kepics, F. Ferrone, and B. Urbanc, *Minimalistic approach to protein assembly modeling / Application to the sickle cell hemoglobin polymerization*, poster presentation, Biophysical Society 55th Annual Meeting, Baltimore, *Biophys. J.* **100**, 389-389 (2011).
29. B. Urbanc, B. Barz, M. Betnel, L. Cruz, G. Bitan and, D. B. Teplow, *Structural basis for amyloid β -protein toxicity inhibition: A multiscale computational study*, poster presentation, Biophysical Society 55th Annual Meeting, Baltimore, *Biophys. J.* **100**, 390-390 (2011).
28. B. Urbanc, B. Barz, M. Betnel, L. Cruz, G. Bitan, and D.B. Teplow, *Elucidation of amyloid β -protein oligomerization pathways in the absence and presence of toxicity inhibitors: Multiscale computational study*, oral presentation, Society for Neuroscience Annual Meeting, Neuroscience 2010, San Diego.
27. B. Barz and B. Urbanc, *All-atom molecular dynamics stability study of amyloid β -protein (1-40) and (1-42) dimers relevant to Alzheimer's disease*, poster presentation, Biophysical Society 54th Annual Meeting, San Francisco, February 2010.

26. L. Cruz, D. B. Teplow, and B. Urbanc, *Computational study of intermediate structures in the folding nucleus of the amyloid β -protein*, oral presentation, Society for Neuroscience Annual Meeting, Neuroscience 2009, Chicago.
25. M. Betnel, L. Cruz, B. Wolozin, and B. Urbanc, *Computational studies of protein folding and aggregation in Parkinson's disease*, poster presentation, Fall American Chemical Society Meeting, Washington DC, Abstracts of papers of the ACS Meeting **238**, Meeting Abstract: 586-PHYS (2009).
24. M. Betnel, L. Cruz, B. Wolozin, and B. Urbanc, *Computational study of α -synuclein protein folding and assembly in Parkinson's disease*, poster presentation, Protein Society Meeting, Boston, July 2009.
23. G. Bitan, H. Li, S. Sinha, A. Attar, R. Bakshi, T. Schrader, P. Talbiersky, J. Polkowska, T. Gersthagen, G. Benedek, A. Lomakin, C.-W. Xie, M. Tan, B. Urbanc, L. Cruz, S. Frautschy, F. Yang, S. Hu, D. Gant, M. Bowers, M. Murray, J.-E. Shea, and C. Wu, *Rationally designed inhibitors of amyloid β -protein assembly and toxicity*, poster presentation, 9th International Conference on AD/PD, Prague, March 2009.
22. B. Urbanc, L. Cruz, A. Lam, G. Bitan, and D. B. Teplow, *Computational Study of Assembly and Toxicity Inhibition of Amyloid β -Protein and Its Arctic Mutant*, 53rd Annual Meeting of Biophysical Society, oral presentation, Session "Amyloids from Multiple Perspectives," Boston, *Biophys. J.* **96**, 219, 2009.
21. B. Urbanc, L. Cruz, and G. Bitan, *Effects of peptide inhibitors and Met35 oxidation on amyloid β -protein oligomerization: In vitro driven computational study*, oral presentation, Slide Session 115.7 of "Alzheimer's Disease: A β Assembly and Deposition I," *The 37th Annual Meeting of the Society for Neuroscience*, San Diego, 3-7 November 2007.
20. B. Urbanc, L. Cruz, and G. Bitan, *In silico study of amyloid β -protein aggregation in the presence of peptide inhibitors*, poster presentation, *The 21th Symposium of the Protein Society*, Boston, Massachusetts, July 21-25, 2007.
19. B. Urbanc, R. Bansil, and B. Turner, *Folding and Aggregation of Mucin Domains*, oral presentation, APS March Meeting, Abstract #**B24.009**, 24009, 2007.
18. B. Urbanc, L. Cruz, and G. Bitan, *Oligomerization of amyloid β -protein with oxidized Met³⁵: A discrete molecular dynamics study*, poster presentation, *The 21th Symposium of the Protein Society*, Boston, Massachusetts, July 21-25, 2007.
17. S. J. Yun, B. Urbanc, L. Cruz, G. Bitan, D. B. Teplow, and H. E. Stanley, *Role of electrostatic interactions in amyloid β -protein (A β) oligomer formation: A discrete molecular dynamics study*, poster presentation, *Biophys. J.*, Supplement **S**, 195A-195A (2007).
16. B. Urbanc, L. Cruz, E. Fradinger, G. Bitan, D. B. Teplow, and H. E. Stanley, *Computational study of amyloid β -protein oligomerization in the presence of C-terminal fragments*, poster presentation (**168.15**), *A Society for Neuroscience 2006 Annual Meeting* (15 October, 2006), Atlanta.
15. S. M. Spring, S. L. Bernstein, N. D. Lazo, B. Urbanc, H. E. Stanley, M. T. Bowers, D. B. Teplow, and G. Bitan, *Towards inhibition of amyloid β -protein oligomerization*, poster presentation, *Understanding Biology Using Peptides*, Sylvie E. Blondelle (Ed.), 19th American Peptide Society Symposium, San Diego, California, Proceedings, 515–516 (2005).
14. S. Peng, B. Urbanc, F. Ding, L. Cruz, S. V. Buldyrev, N. V. Dokholyan, and H. E. Stanley, *Multi-layer Parallel β -Sheet Structure of Amyloid β Peptide (1-40) Aggregate Observed by Discrete Molecular Dynamics Simulations*, poster presentation, APS March Meeting Abstracts, page 1284, 2003.
13. B. T. Hyman, R. B. Knowles, C. Wyart, S. V. Buldyrev, L. Cruz, B. Urbanc, M. E. Hasselmo, and H. E. Stanley, meeting abstract *Plaque-induced neurite abnormalities: Implications for disruption of neural networks in Alzheimer's disease*, poster presentation, *J. Neuropath. Exp. Neurol.* **58** 557-557, 1999.
12. R. B. Knowles, L. Cruz, B. Urbanc, R. H. Christie, H. E. Stanley, and B. T. Hyman, meeting abstract, *The effect of senile plaques and neuropil threads on neurite morphology in Alzheimer's disease*, poster presentation, *Neurology* **48**, 3045–3045 Suppl. 2, 1997.
11. B. Kutnjak-Urbanc, S. Havlin and H. E. Stanley, *Temporal correlations in a one-dimensional sandpile model*, oral presentation, Material Research Science (MRS) Fall Meeting, Boston (Abstract M11.8), 1995.
10. B. Kutnjak-Urbanc, S. Zapperi, S. Milošević and H. E. Stanley, *Sandpile model on Sierpinski gasket fractal*, oral presentation, Gordon Conference "Condensed Matter Physics," Brewster Academy, New Hampshire, 1995.

9. B. Kutnjak-Urbanc and B. Žekš, *Microscopic origin of spontaneous polarization in ferroelectric SmC* liquid crystals, poster presentation*, 15th International Conference on Liquid Crystals, Budapest, Hungary, 1994.
8. B. Kutnjak-Urbanc, S. Zapperi, S. Milošević and H. E. Stanley, *Sandpile model on Sierpinski gasket fractal, oral presentation*, Gordon Conference "Condensed Matter Physics," Brewster Academy, New Hampshire, 1995.
7. B. Kutnjak-Urbanc and B. Žekš: *Phase Transition in Ferroelectric Liquid Crystals Induced by an Electric Field, poster presentation*, NATO Advanced Study Institute "Phase Transitions and Relaxation in Systems with Competing Energy Scales," Geilo, Norway, 1993.
6. B. Kutnjak-Urbanc and B. Žekš: *Phason Spectrum of Ferroelectric Liquid Crystals in an External Electric Field, poster presentation*, European Conference on Liquid Crystals, Flims, Switzerland, 1993.
5. I. Drevenšek, M. Čopič, B. Kutnjak-Urbanc, and B. Žekš: *Nonlinear optical susceptibility of ferroelectric liquid crystals, poster presentation*, 14th International Liquid Crystal Conference, Pisa, Italy, 1992.
4. B. Kutnjak-Urbanc, B. Žekš, and B. Rovšek: *Unwinding of the helical structure of the SmC* phase in external magnetic and electric fields, poster presentation*, 14th International Liquid Crystal Conference, Pisa, Italy, 1992.
3. B. Kutnjak-Urbanc and B. Žekš: *The Phase Diagram of Ferroelectric Liquid Crystals in the External Magnetic Field, poster presentation*, European Conference on Liquid Crystals, Courmayeur, Italy, 1991.
2. B. Kutnjak-Urbanc and B. Žekš: *Influence of Static Electric and Magnetic Fields on Optical Properties of Ferroelectric Liquid Crystals, poster presentation*, III. International Topical Meeting on Optics of Liquid Crystals, Cetraro, Italy, 1990.
1. B. Kutnjak-Urbanc and B. Žekš: *The Microscopic Origin of the Polarization in Ferroelectric Liquid Crystals, oral presentation*, "The Molecular Dynamics of Liquid Crystals," NATO Advanced Study Institute, Il Ciocco, Italy, 1989.

RESEARCH PUBLICITY

- The online news commentary entitled, *Flexible N-Termini Key to A β Oligomer Toxicity?* by Alzforum writer Esther Landhuis comments on computational results of my group that were presented at Neuroscience 2010, 40th annual meeting of the Society for Neuroscience in San Diego in November 2010.
- Biophysics Group of Drexel University's Physics Department was featured in the August 2009 issue of the APS Division of Biological Physics Newsletter "The Biological Physicist". Professors Luis Cruz Cruz, Frank Ferrone, Brigita Urbanc, Guoliang Yang, and Jian-Min Yuan were interviewed by Dr. Sonya Bahar.
- The findings contained in "Publications" (Ref. [33]) that appeared in the *Proceedings of the National Academy of Science* on November 9, 2004, regarding the loss of microcolumnar strength as a function of age in area 46 of rhesus monkey brains, were reviewed in the AAAS Science on-line publication *Science of Aging Knowledge Environment*, **2004** Iss. 45, pp. nf100, November 10, 2004. The review article was entitled "Out of Whack, Out of Mind" and was written by M. Leslie. In addition, these scientific findings were reviewed in an article that appeared in the *NCRR Reporter XXVIII*, No. 4 (2004), a quarterly magazine of the National Center for Research Resources of the NIH. The article was entitled "Aging Neurons on the Move," and was written by Tina Adler.
- The findings contained in "Publications" (Ref. [27]), that appeared in the *Proceedings of the National Academy of Science* on May 9, 2000 were reviewed on a column in *BioWorld Today*, **11** No. 76, April 20, 2000, under the title "Physicists Correlate Neuronal Die-Off in Alzheimer's Patients with Cortical Columnar Damage," by their science editor, David N. Leff. *BioWorld Today* is a newspaper for the biotechnology industry. It is faxed every day to leading biotechnology professionals and investors with high impact in Wall Street and the business world in general. In addition, the main figure illustrating the findings of the microcolumnar organization of neurons in the brain won the honor to be featured on the cover of the May 9th issue of the *Proceedings of the National Academy of Science* with an invited commentary.
- The mathematical model with the corresponding clinical consequences contained in "Publications" (Ref. [21]) published in the *Proceedings of the National Academy of Science*, Vol. 94, in 1997 were reviewed on the fall edition of *Bostonia* in 1997. The feature article was entitled "Unraveling Alzheimer's" and was written by their managing editor, Taylor McNeil.

PHYSICS EDUCATION RESEARCH

- Coordinator of the “Water and Molecular Networks” education project on teaching science at high-school and undergraduate levels via the use of computers. Responsibilities: development of a written manual for high school and college students, which accompanied the molecular dynamics simulation software for visualization of random motion phenomena. Boston University, 1996–1998.
- Coordinator of the hands–on experiments for the “Water and Molecular Networks” education project, which introduced several topics ranging from percolation to granular materials in an intuitive and visual way in order to bridge the gap in understanding between microscopic and the macroscopic phenomena. Responsibilities: development of curriculum materials for chemistry, physics, and biology high school courses using simple hands–on activities, including wet–lab experiments. Boston University, Summer 1994 - Summer 1996.

TEACHING

DREXEL UNIVERSITY

UNDERGRADUATE COURSES

- *Fundamentals of Physics I, PHYS 101*
Fall Quarter 2010-11, Course Director; Winter Quarter 2012-13, Instructor; Winter Quarter 2013-14, Instructor; Fall Quarter 2014-15, Course Director; Winter Quarter 2014-15, Instructor; Winter Quarter 2016-17, Course Director
- *Fundamentals of Physics II, PHYS 102*
Spring Quarter 2012-13, Instructor; Spring Quarter 2013-14, Instructor; Spring Quarter 2014-15, Instructor; Spring Quarter 2016-17, Instructor; Winter Quarter 2017-18, Course Director; Spring Quarter 2018-19, Instructor
- *Fundamentals of Physics III, PHYS 201*
Winter Quarter 2008-09, Course Director; Winter Quarter 2009-10, Course Director; Winter Quarter 2010-11, Course Director; Winter Quarter 2011-12, Course Director; Fall Quarter 2012-13, Course Director; Spring Quarter 2010-11, Course Director; Spring Quarter 2011-12; Course Director; Fall Quarter 2016-17, Course Co-Director; Spring Quarter 2017-18; Course Director
- *Thermodynamics, PHYS 217*
Fall Quarter 2016-17, Course Director; Fall Quarter 2017-18, Course Director; Fall Quarter 2018-19, Course Director; Fall Quarter 2019-20, Course Director; Fall Quarter 2020-21, Course Director
- *Electromagnetic Fields II, PHYS 322*
Winter Quarter 2018-19, Course Director
- *Senior Research I, PHYS 491*
Fall Quarter 2015-16, Course Director; Fall Quarter 2020-21, Course Director
- *Senior Research II, PHYS 492*
Winter Quarter 2020-21, Course Director
- *Senior Research III, PHYS 493*
Spring Quarter 2019-20, Course Director; Spring Quarter 2020-21, Course Director

UNDERGRADUATE & GRADUATE COURSES

- *Guest Lecture, BIO 415-615*
Molecular Dynamics Simulations of Proteins, by invitation by the Course Director, Prof. Joe Benz; Spring 2011; Spring 2012; Spring 2013

- *Biophysics, PHYS 461-561*
Fall Quarter 2009-10, Course Director; Fall Quarter 2011-12, Course Director; Fall Quarter 2013-14, Course Director;
Fall Quarter 2015-16, Course Director; Fall Quarter 2017-18, Course Director; Fall Quarter 2019-20, Course Director;
Fall Quarter 2021-22, Course Director
- *Statistical Mechanics I, PHYS 521*
Winter Quarter 2021-22, Course Director
- *Statistical Mechanics II, PHYS 522*
Spring Quarter 2021-22, Course Director

BOSTON UNIVERSITY

- *Elementary Modern Physics, PY 313*
Summer I 2006, Course Director; Spring Semester 2008, Course Co-Director
- *PY 482, Guest Seminar*
Statistical Physics Approach to Understanding Alzheimer's Disease, October 2006
- *PY-105, Guest Lecture*
Applications of Newtonian Mechanics to Understand Molecular Basis of Alzheimer's Disease: A Molecular Dynamics Study of Protein Folding and Aggregation, March 2007
- *PY 482, Guest Seminar*
Discrete Molecular Dynamics Study of Alzheimer's Amyloid β -Protein Assembly, February 2008

UNIVERSITY OF LJUBLJANA, SLOVENIA

- *Physics for Mathematics Majors*
Teaching Assistant, Department of Physics, 1987–1996.

RESEARCH DIRECTING AND ADVISING

UNDERGRADUATE TRAINEES

In the following, STAR stands for *Students Tackling Advanced Research*, a program offered at Drexel University to encourage freshmen undergraduates to participate in research activities.

- **Thomas Ruggiero**, Department of Physics, REU & co-op (Spring and Summer Quarters 2020-21). Research: Molecular dynamics simulations of $A\beta$ -membrane interactions and short unfolded peptides in water. Supported by NSF grants OAC-1919691 (Amendment ID 001) and NSF MCB-1817650. Role: Research Advisor.
- **Kausheya Basu**, Department of Physics, Senior Thesis Research (Fall, Winter, and Spring Quarter 2019-20). Research: Modeling a lipid bilayer using four beads per lipid by discrete molecular dynamics. Received B.S. in 2020. Role: Research Advisor.
- **Sarah Adams**, Department of Physics, Senior Thesis Research Student (Fall, Winter, and Spring Quarter 2018-19). Research: She analyzed the phase diagram of GAG self-assembly obtained from discrete molecular dynamics simulations. Senior Thesis Title: *Discrete Molecular Dynamics Study of GAG Aggregation*. Received B.S. in 2019. Role: Research Advisor.
- **Joshua Weisberg**, Department of Physics, STAR Student (Summer Quarter 2017-18). Research: Exploration of the three-bead (Cooke-Deserno) lipid model of a membrane by discrete molecular dynamics. Role: Research Advisor.
- **Cuong (Ken) Trinh**, Department of Physics, Co-op Student (06/18/2018–06/15/2019). Research: Analysis of molecular dynamics trajectories of GAG self-assembly in ethanol/water mixtures. Role: Research Advisor.

- **Stephen Windle**, Department of Physics, Volunteering Student (09/01/2017–06/30/2018). Research: Statistical analysis of the arrangement of amino acid residues within proteins using protein databases. Role: Research Advisor.
- **Kausheya Basu**, Department of Physics, STAR Student (Summer Quarter 2016-17). Research: Modeling a lipid bilayer using Cooke-Deserno model and discrete molecular dynamics: Visualization of a lipid bilayer in VMD. Role: Research Advisor.
- **Riley Stanford**, Department of Physics, Volunteering Student (12/01/2014–03/31/2017). Research: Structural analysis of oligomers formed by the Osaka mutants of $A\beta_{40}$ and $A\beta_{42}$. Role: Research Advisor.
- **Akihito Tomida**, Department of Physics, Senior Thesis Research Student (AY 2013-14). Received B.S. in 2014. Senior Thesis Title: *The effect of amino acid substitutions at position 2 on $A\beta$ folding and oligomer formation*. Role: Research Advisor.
- **Nick Kruczek**, Department of Physics, Senior Thesis Research Student (AY 2012-13). Received B.S. in 2013. Senior Thesis Title: *The effect of amino acid substitutions K16A and K28A on amyloid β -protein self-assembly*. Role: Research Advisor. Current Position: Graduate student of astrophysics at the University of Colorado Boulder.
- **Dillion M. Fox**, Department of Physics, Volunteering and STAR Student (01/08/2012–02/27/2013). Research: The effect of cross-linking on amyloid β -protein oligomer formation and structure. Role: Research Advisor. Current Position: Graduate student of biophysics at University of Pennsylvania.
- **Peter Massey**, Department of Biology, Co-op and Volunteering Student (AY 2010-11 and AY 2011-12). Research: Exploring the effect of F4G substitution on amyloid β -protein oligomer formation. Role: Research Advisor.
- **Brian Cohen**, Department of Physics, Co-op Student (Spring and Summer Quarters of AY 2010-11). Research: Calculation of cross-correlations between neurons and amyloid plaques in a transgenic mouse model of Alzheimer's disease. Role: Research Advisor.
- **Chris Kepics**, Department of Physics, Co-op Student (Spring and Summer Quarters of AY 2009-10). Research: Discrete molecular dynamics simulations of a minimal model of self-assembly. Role: Research Advisor.

GRADUATE TRAINEES (Ph.D. and Postdoctoral)

DREXEL UNIVERSITY

- **Athul (Ash) Suresh**, PhD student, Department of Physics (09/01/2021–present). Research: Assessment and experiment-based modifications of the molecular dynamics force field. Supported in part by the NSF grant NSF MCB-1817650. Role: PhD Thesis Advisor.
- **Rachit Pandey**, PhD student, Department of Physics (09/01/2021–present). Research: Analysis of oligomer formation of distinct physiologically-relevant C-terminal variants of amyloid β -protein examined by discrete molecular dynamics. Role: PhD Thesis Advisor.
- **Riya Shah**, MS student, Department of Physics (09/01/2020–07/01/2022). Research: Analysis of discrete molecular dynamics simulations of self-assembly of the Osaka mutants of $A\beta$ peptides and fully-atomistic simulations of short linear motifs in water. Supported in part by the NSF grant NSF MCB-1817650. Received MS in 2022. Thesis Title: *The effect of Osaka mutation on oligomer formation of full-length amyloid β -protein*. Role: MS Thesis Advisor.
- **Brian Andrews**, PhD student, Department of Physics (09/01/2018–present). Research: Discrete molecular dynamics simulations of villin headpiece assembly. Calibration of molecular dynamics force field based on experimental constraints of GxG in water. Supported in part by the NSF grant NSF MCB-1817650. Role: Research Advisor.
- **Andrew Antczak**, PhD student, Department of Physics (09/01/2017–08/15/2019). Research: Discrete molecular dynamics simulations of assembly of lipids into a bilayer. Received M.S. in 2019. Role: Research Advisor.
- **Blake Antos**, PhD student, Department of Physics (09/01/2015–01/31/2018). Research: Computational biophysics of lipid self-assembly. Received M.S. in 2017. Role: Research Advisor.

- **Shuting Zhang**, PhD student, Department of Physics (09/24/2015–09/05/2020). Research: Computational studies of the effect of cross-linking on amyloid β -protein oligomer formation and structure. Molecular dynamics studies of short unfolded peptides and force field development. Received Ph.D. in 2020. Thesis Title: *Molecular Dynamics of Amyloid β -Protein Assembly under Oxidative Conditions and Short Peptides in Aqueous Solutions*. Role: Ph.D. Thesis Advisor.
- **Kaho Long**, PhD student, Department of Physics (09/24/2015–12/17/2019). Research: Experimental studies of insulin at neutral pH, its effect on membrane integrity of biomimetic lipid vesicles, and its interaction with amyloid β -protein. Received Ph.D. in 2019. Thesis Title: *The effect of insulin on self-assembly and toxicity of amyloid β -protein: Implications to type 2 diabetes and Alzheimer's disease*. Role: PhD. Thesis Advisor.
- **Matthew T. Mawhinney**, PhD student, Department of Physics (09/01/2011–09/15/2017). Research: (i) *In vitro* characterization of insulin oligomers at neutral and low pH and (ii) Characterization of CTCF-induced DNA morphologies by atomic force microscopy. Received Ph.D. in 2017. Thesis Title: *Protein self-assembly and protein-induced DNA morphologies*. Role: Ph.D. Thesis Advisor.
- **Matthew J. Voelker**, PhD student, Department of Physics (09/01/2011–09/15/2017). Research: Computational study of porelike morphologies formed by amyloid β -protein and α synuclein. Received Ph.D. in 2017. Thesis Title: *Porelike morphologies in amyloidogenic proteins*. Role: Ph.D. Thesis Advisor. Current Position: Product Support Engineer at OSIsoft.
- **Derya Meral**, PhD student, Department of Physics (09/01/2008–09/15/2015). Research: Molecular dynamics simulations of unfolded and intrinsically disordered peptides. Received Ph.D. in 2015. Thesis Title: *Molecular dynamics studies of intrinsically disordered peptides and proteins*. Role: Ph.D. Thesis Advisor.
- **Ian Eaves**, PhD student, Department of Physics (09/01/2011–12/31/2014). Research: Computational biophysics of amyloid β -protein. Received M.S. in 2014. Current Position: Data Scientist at CiBO Technologies, Greater St. Louis Area.
- **Runcong Liu**, PhD student, Department of Physics (09/01/2006–08/31/2012). Research: Atomic force microscopy of CTCF-induced DNA complexes. Received Ph.D. in 2012. Thesis Title: *Investigation of the interaction between CTCF and DNA using AFM imaging*. Role: Ph.D. Thesis Advisor (09/01/2011–08/31/2012), after Dr. Guoliang Yang, who was Runcong Liu's initial Ph.D. advisor, passed away.)
- **Nicole Wagner**, PhD student, Department of Physics (09/01/2010–12/31/2012). Research: Experimental biophysics of insulin. Current Position: Research Assistant at Georgetown University, Washington D.C.
- **Thomas L. Williams, PhD**, Postdoctoral fellow (09/01/2011–09/01/2013). Research: Experimental studies of protein aggregation and its effect on the integrity of biomimetic lipid vesicles. Current Position: Practice Consultant at Clarivate Analytics.
- **Bogdan Barz, PhD**, Postdoctoral fellow, Department of Physics (10/01/2009–07/30/2012). Research: Computational biophysics of protein folding and assembly. Role: Research Advisor. Current Position: Young Investigator, Forschungszentrum Jülich, Germany.
- **Yuriy V. Sereda, PhD**, Postdoctoral fellow, Department of Physics (09/01/2009–06/30/2010). Research: Implementation of proline-specific force field into the four-bead protein discrete molecular dynamics model.

BOSTON UNIVERSITY

- **Mark Betnel**, Department of Physics (09/01/2005–12/15/2010). Research: Computational biophysics of amyloid β -protein and α synuclein. Received Ph.D. in 2010. Thesis Title: *From misfolded proteins to soluble oligomers and beyond: discrete molecular dynamics in the study of Alzheimer's and Parkinson's diseases*. Role: Ph.D. Thesis Advisor. Current Position: Science Teacher at Seattle Academy of Arts and Sciences Greater Seattle Area.

UNIVERSITY OF LJUBLJANA, SLOVENIA

- **Matjaž Žganec**, Department of Physics (2010–2017). Research: Discrete molecular dynamics studies of stefin B self-assembly. Role: Research Advisor; Co-Advisor: Dr. Eva Žerovnik (Institute Jožef Stefan, Ljubljana, Slovenia).

GRADUATE STUDENTS VISITING FROM OTHER UNIVERSITIES

- **Meng Sun**, Department of Physics (AY 2013-14). Ph.D. candidate at Temple University. Research: Discrete molecular dynamics simulations using a coarse-grained model of hemoglobin.
- **Chetan Poojari**, Department of Physics (02/2012 - 05/2012). Ph.D. candidate in the group of Birgit Strödel at Forschungszentrum Jülich, ICS-6: Structural Biochemistry (Germany). Research: Development of a coarse-grained lipid model for discrete molecular dynamics simulations.

SERVICE

DREXEL UNIVERSITY

- Associate Department Head of Graduate Studies, Department of Physics, 09/01/2020–present.
- Acting Associate Department Head of Graduate Studies, Department of Physics, 09/01/2019–08/31/2020.
- University Research Computing Facility (URCF) Board Member, 2017–2020.
- *Interim* Director of Graduate Admissions, Department of Physics, 01/01/2013–08/31/2013.
- Faculty Advisor of *Women in Physics Society*, Department of Physics, 2011–present.

SCIENTIFIC AND BROADER IMPACT COMMUNITY

PROFESSIONAL MEMBERSHIPS

- American Physical Society, 2014–present (lifetime member).
- American Chemical Society, 2009–present (on and off).
- Biophysical Society, 2007–present (on and off).
- Society for Neuroscience, 2006–present (on and off).

SCIENTIFIC AND EDITORIAL BOARDS

- Editorial Board Member of *Biomolecules*, 2020–present.
<https://www.mdpi.com/journal/biomolecules/editors>
- Editorial Board Member of *Journal of Biological Physics*, 2010–present.
<http://link.springer.com/journal/10867>
- Scientific Advisory Board, Alzheimer Research Forum, 2008-2009.
<http://www.alzforum.org>

PARTICIPATION IN ROUNDTABLES AND FAIRS

- APS Virtual Career Fair for Graduate School Applicants, 13-15 September 2021 (12:00-3:00 pm each day).
- Invited roundtable of Directors-of-Graduate-Studies, APS Innovation Fund Project on Graduate Admissions in COVID-19 Era, Pls: Geoff Potvin (Florida International University), Galen Pickett (CSU-Long Beach), Chris Porter (Ohio State University), 60-min meeting on 09/14/2021.
- JoBP GoToMeeting with Sonya Bahar (Editor-in-Chief) and Davide Migliorini (Associate Editor Journals at Springer Nature) on spearheading monthly virtual talks as JoBP Webinar Series, 1-hour meeting on 10/26/2020.
- Invited roundtable of Directors-of-Graduate-Studies, APS Innovation Fund Project on Graduate Admissions in COVID-19 Era, Pls: Geoff Potvin (Florida International University), Galen Pickett (CSU-Long Beach), Chris Porter (Ohio State University), 90-min meeting on 07/28/2020.

INVITED BOOK REVIEWS

1. **Brigita Urbanc**, *Protein Actions: Principles & Modeling*, by I. Bahar, R. L. Jernigan, and K. A. Dill, invited book review, *J. Biol. Phys.* **43**, 585-589 (2017).

AD HOC MANUSCRIPT PEER REVIEWS (journal names listed alphabetically)

- ACS Chemical Neuroscience.
- Acta Neuropathologica.
- Analytica Chimica Acta.
- Angewandte Chemie.
- Biochimica et Biophysica Acta.
- Biochemistry.
- Biomolecules.
- Biophysical Journal.
- Biopolymers.
- Cell Biology and Biophysics.
- Chemical Physics Letters.
- Chemical Science.
- ChemPhysChem.
- Current Biotechnology.
- European Biophysics Journal.
- European Physical Journal B.
- FEBS Journal.
- Future Medicinal Chemistry.
- Future Neurology.
- International Journal of Molecular Sciences.
- iScience.

- ISRN Biomathematics.
- Journal of American Chemical Society.
- Journal of Biological Chemistry.
- Journal of Biological Physics.
- Journal of Chemical Physics.
- Journal of Chemical Information and Modeling.
- Journal of Chemical Theory and Computation.
- Journal of Molecular Biology.
- Journal of Molecular Cell Biology.
- Journal of Physical Chemistry.
- Journal of Physical Chemistry Letters.
- Journal of the Royal Society Interface.
- Molecular Informatics.
- Molecular Neurodegeneration.
- Molecules.
- Nanoscale.
- Nature Communications Chemistry.
- Neuroscience Letters.
- New Journal of Chemistry.
- Peer J.
- Physica A.
- Physical Chemistry Chemical Physics.
- Physical Review E.
- Physical Review Letters.
- Physics Today.
- Phytochemistry.
- PLoS Computational Biology.
- PLoS ONE.
- Polymers.
- Proteins: Structure, Function, and Bioinformatics.
- Royal Society of Chemistry Advances.
- Science.
- Scientific Reports.
- The Open Biochemistry Journal.

AD HOC AND PANEL PROPOSAL REVIEWS

- NSF Panel, Molecular Biophysics Cluster, reviewed 6 proposals, Program Director: Jarek Majewski (6-8 June 2022).
- NSF Ad Hoc CAREER proposal review, Molecular Biophysics, Program Director: Wilson Francisco (24 September 2021).
- NIH Panel Review, Center for Scientific Review, Macromolecular Structure and Function D (MSFD) Study Section, Ian F. Thorpe, Scientific Review Officer, 2-day virtual meeting, **reviewed 9 proposals** (June 16-17, 2021).
- NSF CHE - Macromolec/Supramolec/Nano (Jong In-Hahn, 02/12/2020).
- NSF Materials Innovation Platforms (MIP) & National Facilities and Instrumentation (NaFI), Division of Materials Research (DMR): two MIP proposals (09/13/2019).
- Netherlands Organisation for Scientific Research (NWO) grant application (12/10/2018).
- NSF Molecular and Cellular Biophysics (MCB) Career Panel Meeting, Alexandria, VA 22314 (18-19 September 2018).
- Medical Research Council, UK (March 2018).
- French National Research Agency (Agence National de la Recherche, ANR), AlzLux grant proposal (May 2016).
- Netherlands Organisation for Scientific Research, Council for the Earth and Life Sciences (October 2014).
- NASA Research Opportunities in *Complex Fluids and Macromolecular Biophysics*, Panel Meeting, NASA Research and Education Support Services, Arlington, VA (June 2013).
- University of Maryland, Maryland Industrial Partnerships (MIPS) (November 2012).
- European Research Council, Brussels (March 2012).
- Neurological Foundation New Zealand (November 2011).
- NSF (March 2010, March 2011, June 2012, April 2013, March 2014).

INVITED COMMENTARIES ON THE WEB (in reverse chronological order)

22. For www.alzforum.org commentary on the research paper by Cohen S. A., Cukalevski R., Michaels T. C., Šarić, A., Törnquist M., Vendruscolo M., Dobson C. M., Buell A. K., Knowles T. P., Linse S. *Distinct thermodynamic signatures of oligomer generation in the aggregation of the amyloid- β peptide* Nat. Chem. 2018. Commentary posted on 26 March 2018 at:
<https://www.alzforum.org/papers/distinct-thermodynamic-signatures-oligomer-generation-aggregation-amyloid-v-peptide#comment-26836>
21. For www.alzforum.org commentary on the research paper by R. Gallardo1, M. Ramakers, F. De Smet, F. Claes, L. Khodaparast, L. Khodaparast, José R. Couceiro, T. Langenberg, M. Siemons, S. Nyström, L.J. Young, R.F. Laine, L. Young, E. Radaelli, I. Benilova, M. Kumar, A. Staes, M. Desager, M. Beerens, P. Vandervoort, A. Luttun, K. Gevaert, G. Bormans, M. Dewerchin, J. Van Eldere, P. Carmeliet, G. Vande Velde, C. Verfaillie, C.F. Kaminski, B. De Strooper, P. Hammarström, K.P.R. Nilsson, L.Serpell, J. Schymkowitz, and F. Rousseau, *De novo design of a biologically active amyloid* Science 2016 Nov 11 [Epub ahead of print]. Commentary posted on 11 November 2016 at:
<http://www.alzforum.org/news/research-news/amyloid-deposits-not-always-toxic-cells#comment-22311>
20. For www.alzforum.org commentary on the research paper by Schmidt M., Rohou A., Lasker K., Yadav J.K., Schiene-Fischer C., Fändrich M., and Grigorieff N. *Peptide dimer structure in an A β (1-42) fibril visualized with cryo-EM*, Proc. Natl. Acad. Sci. USA. 2015 Sep 8 [Epub ahead of print]. Commentary posted on 18 September 2015 at:
<http://www.alzforum.org/news/research-news/electron-microscope-yields-finer-structure-synuclein-av-fibrils#comment-18676>
19. Interviewed by Alzheimer's Research Forum (www.alzforum.org) to comment on research news from Dr. Ishii's group in the story entitled, *Danger, S-Bends! New Structure for A β 42 Fibrils Comes into View*,
<http://www.alzforum.org/news/research-news/danger-s-bends-new-structure-av42-fibrils-comes-view>

18. For www.alzforum.org commentary on the research paper by Fang YS, Tsai KJ, Chang YJ, Kao P, Woods R, Kuo PH, Wu CC, Liao JY, Chou SC, Lin V, Jin LW, Yuan HS, Cheng IH, Tu PH, Chen YR. *Full-length TDP-43 forms toxic amyloid oligomers that are present in frontotemporal lobar dementia-TDP patients*. Nat Commun. 2014 Sep 12;5:4824. Commentary posted on 3 October 2014 at:
<http://www.alzforum.org/papers/full-length-tdp-43-forms-toxic-amyloid-oligomers-are-present-frontotemporal-lobar-dementia>
17. Interviewed by Alzheimer's Research Forum (www.alzforum.org) to comment on research news from Dr. Knowles's group:
<http://www.alzforum.org/new/detail.asp?id=3504>
16. Interviewed by Alzheimer's Research Forum (www.alzforum.org) to comment on research news from Dr. Tycko's group:
<http://www.alzforum.org/new/detail.asp?id=3094>
15. For www.alzforum.org research news entitled, *X-raying A β Oligomers, Unraveling Mysteries of Amyloid Aggregation*, based on paper by Streltsov VA, Varghese JN, Masters CL, Nuttall SD. "Crystal structure of the amyloid- β p3 fragment provides a model for oligomer formation in Alzheimer's disease," J Neurosci. 2011 Jan 26;31(4):1419-26. News on 2 February 2011, published on-line at:
<http://www.alzforum.org/new/detail.asp?id=2679>
14. For *The Scientist* on new research in aging dementia (S. Peleg *et al.*, "Altered histone acetylation is associated with age-dependent memory impairment in mice," Science **328**, 753-756, 2010.) **Epigenetic change ups dementia?** published on-line at:
<http://www.the-scientist.com/blog/display/57396/>
13. For *The Scientist* on Alzheimer's disease research news (Jang *et al.*, "Truncated β -amyloid peptide channels provide an alternative mechanism for Alzheimer's Disease and Down syndrome," PNAS Early Edition, March 2010), **Alzheimer's drugs hurt brain?**, published on-line at:
<http://www.the-scientist.com/blog/display/57251/>
12. For www.alzforum.org on research paper by Bleiholder C., Dupuis N.F., Wyttenbach T., Bowers M.T. "Ion mobility–mass spectrometry reveals a conformational conversion from random assembly to β -sheet in amyloid fibril formation," Nature Chemistry 2010 Dec 19. Comment on 5 January 2011, published on-line at:
<http://www.alzforum.org/pap/annotation.asp?powID=112357#{8B904250-DDCB-40F7-9C76-14EEE4DCD0D4}>
11. For www.alzforum.org on research news entitled, *The Toxic Fold? A β Dodecamers, Tetramers Show Their Conformations*, based on the papers by Bernstein SL, Dupuis NF, Lazo ND, Wyttenbach T, Condrón MM, Bitan G, Teplow DB, Shea J, Ruotolo BT, Robinson CV, Bowers MT. Amyloid- β protein oligomerization and the importance of tetramers and dodecamers in the aetiology of Alzheimer's disease. Nature Chemistry. 2009 & Clemmer DE, Valentine SJ. Protein oligomers frozen in time. Nature Chemistry. 2009 & Harmeyer A, Wozny C, Rost BR, Munter LM, Hua H, Georgiev O, Beyermann M, Hildebrand PW, Weise C, Schaffner W, Schmitz D, Multhaup G. Role of amyloid- β glycine 33 in oligomerization, toxicity, and neuronal plasticity. J Neurosci. 2009. 17 June 2009, published on-line at:
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