GIACOMO FIORIN
Curriculum Vitae

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Web profiles:	Scholar OrcID LinkedIn GitHub Webpage

PROFESSIONAI EXPERIENCE

08/2020 – present	Staff scientist, National Institutes of Health
06/2018 – 06/2020	Research collaborator, National Institutes of Health
07/2015 – 07/2020	Associate Professor of Research, Temple University
01/2017 – 06/2018	Contractor, National Institutes of Health
07/2011 – 07/2015	Assistant Professor of Research, Temple University
09/2009 – 06/2011	Postdoctoral Research Associate, Temple University (Advisor: Michael L. Klein)
05/2007 – 08/2009	Postdoctoral Research Associate, University of Pennsylvania (Advisor: Michael L. Klein)

EDUCATION

10/2002 – 12/2006	PhD in Statistical and Biological Physics, International School for Advanced Studies, Trieste, Italy (Advisor: Paolo Carloni)
10/1997 – 02/2002	Combined BS+MS in Physics, University of Padua, Italy (Advisor: Enrico Maglione)

RESEARCH INTERESTS

- Structure and dynamics of biological membranes.
- Free-energy computation and enhanced sampling methods.
- High-performance simulation software for molecular dynamics.
- Self-assembled polymer structures.
- Coarse-grained molecular modeling of macromolecules.
- Numerical integration schemes for molecular-dynamics simulation.

PEER-REVIEWED PUBLICATIONS

(* = equal contribution with others, † = (co-)corresponding authorship).

1. **Fiorin G**†, Forrest LR, Faraldo-Gomez JD.
   "Membrane free-energy landscapes derived from atomistic dynamics explain nonuniversal cholesterol-induced stiffening"
   PNAS Nexus (in press) https://doi.org/10.1093/pnasnexus/pgad269
2. Kawamoto S, Liu H, Miyazaki Y, Seo S, Dixit M, DeVane RH, MacDermaid CM, **Fiorin G**, Klein ML, Shinoda W.
   "SPICA Force Field for Proteins and Peptides"
   J. Chem. Theory Comput. **18**(5):3204-3217 (2022) https://doi.org/10.1021/acs.jctc.1c01207
3. Hénin J, Lopes LJS, **Fiorin G.**
   "Human learning for molecular simulations: the Collective Variables Dashboard in VMD"
   J. Chem. Theory Comput. **18**(3):1945-1956 (2022) https://doi.org/10.1021/acs.jctc.1c01081
4. Finkelstein J, Cheng C, **Fiorin G**, Seibold B, Grønbech-Jensen N.
   "Bringing discrete-time Langevin splitting methods into agreement with thermodynamics"
   J. Chem. Phys. **155**(18):184104 (2021) https://doi.org/10.1063/5.0066008
5. **Fiorin G**†, DelloStritto MJ, Percec S, Klein ML.
   "Shear response in crystalline models of poly(p-phenylene terephthalamide)"
   Mol. Phys. **119**(19-20):e1948122 (2021) https://doi.org/10.1080/00268976.2021.1948122
6. Finkelstein J, Cheng C, **Fiorin G**, Seibold B, Grønbech-Jensen N.
   "The Challenge of Stochastic Størmer-Verlet Thermostats Generating Correct Statistics"
   J. Chem. Phys. **153**(13):134101 (2020) https://doi.org/10.1063/5.0018962
7. Phillips JC, Hardy DJ, Maia JDC, Stone JE, Ribeiro JV, Bernardi RC, Buch R, **Fiorin G**, Hénin J, Jiang W, McGreevy R, Melo MCR, Radak BK, Skeel RD, Singharoy A, Wang Y, Roux B, Aksimentiev A, Luthey-Schulten Z, Kalé LV, Schulten K, Chipot C, Tajkhorshid E.
   "Scalable molecular dynamics on CPU and GPU architectures with NAMD"
   J. Chem. Phys. **153**(4):044130 (2020) https://doi.org/10.1063/5.0014475
8. Yu J, **Fiorin G**, Peng H, Klein ML, Perdew JP.
   "A different bonding type along each crystallographic axis: Computational study of poly-phenylene terephthalamide."
   Phys. Rev. Materials **4**: 055601 (2020) https://doi.org/10.1103/PhysRevMaterials.4.055601
9. MacDermaid CM, Hall KW, DeVane RH, Klein ML, **Fiorin G**†.
   "Coexistence of lipid phases stabilizes interstitial water in the outer layer of mammalian skin."
   Biophys. J. **118**(7):1588-1601 (2020) (Cover article) https://doi.org/10.1016/j.bpj.2020.01.044
10. **Fiorin G**†, Marinelli F, Faraldo-Gómez JD.
    "Direct derivation of free energies of membrane deformation and other solvent density variations from enhanced sampling molecular dynamics."
    J. Comp. Chem. **41**(5):449-459 (2020) https://doi.org/10.1002/jcc.26075
11. Zhou W, **Fiorin G**, Anselmi C, Karimi-Varzaneh HA, Poblete H, Forrest LR, Faraldo-Gómez JD.
    "Large-scale state-dependent membrane remodeling by a transporter protein."
    eLife **8**:e50576 (2019) https://doi.org/10.7554/eLife.50576

12. Finkelstein J, **Fiorin G**†, Seibold B.
"Comparison of modern Langevin integrators for simulations of coarse-grained polymer melts."
Mol. Phys. **118**(6): e1649493 (2020) https://doi.org/10.1080/00268976.2019.1649493
Pre-Print: https://arxiv.org/pdf/1904.00532v1.pdf

13. Mogurampelly S, MacDermaid CM, Percec S, Klein ML, **Fiorin G†.**
"Aggregation of poly(p-phenylene terephthalamide) chains: emergence of fiber defects."
Phys. Rev. Materials **3**: 015602 (2019) https://doi.org/10.1103/PhysRevMaterials.3.015602

14. Marinelli F, **Fiorin G**.
"Structural characterization of biomolecules through atomistic simulations guided by DEER measurements."
Structure **27**(2): 359-370 (2019) https://doi.org/10.1016/j.str.2018.10.013

15. Zhang Z, Mogurampelly S, Percec S, Hu Y, **Fiorin G**†, Klein ML, Ren S.
"Mechanically Strong Polymer Sheets from Aligned Ultrahigh-Molecular-Weight Polyethylene Nanocomposites"
J. Phys. Chem. Lett. **9**(10): 2652-2658 (2018) http://dx.doi.org/10.1021/acs.jpclett.8b00790

16. Markiewicz BN, Lemmin T, Zhang W, Ahmed IA, Jo H, **Fiorin G**, Troxler T, DeGrado WF, Gai F.
"Infrared and fluorescence assessment of the hydration status of the tryptophan gate in the influenza A M2 proton channel."
Phys. Chem. Chem. Phys. **18**(41): 28939-28950 (2016) http://dx.doi.org/10.1039/C6CP03426H

17. MacDermaid CM, Kashyap HK, DeVane RH, Shinoda W, Klauda JB, Klein ML, **Fiorin G**†.
"Molecular dynamics simulations of cholesterol-rich membranes using a coarse-grained force field for cyclic alkanes"
J. Chem. Phys. **143**:243144 (2015) http://dx.doi.org/10.1063/1.4937153

18. Thomaston JL, Alfonso-Prieto M, Woldeyes RA, Fraser JS, Klein ML, **Fiorin G**†, DeGrado WF.
"High resolution structures of the M2 proton channel from influenza A virus reveal dynamic pathways for proton stabilization and transduction."
Proc. Natl. Acad. Sci. USA. **112**(46):14260-14265 (2015) http://dx.doi.org/10.1073/pnas.1518493112

19. Shen R, Han W, **Fiorin G**, Islam SM, Schulten K, Roux B.
"Structural Refinement of Proteins by Restrained Molecular Dynamics Simulations with Non-interacting Molecular Fragments"
PLOS Comput Biol **11**(10):e1004368 (2015) http://dx.doi.org/10.1371/journal.pcbi.1004368

20. Oh KI, **Fiorin G**, Gai F.
"How Sensitive Is the Amide I Vibration of the Polypeptide Backbone to Electric Field?"
Chem Phys Chem, http://dx.doi.org/10.1002/cphc.201500777

21. MacDermaid CM, DeVane RH, Klein ML, **Fiorin G**†.
"Dehydration of multilamellar fatty acid membranes: a molecular dynamics-based model for skin acidification"
J. Chem. Phys. **141**:22D526 (2014) http://dx.doi.org/10.1063/1.4902363

22. Gianti E, Carnevale V, DeGrado WF, Klein ML, **Fiorin G**†.
"Hydrogen-bonded water molecules in the M2 channel of the influenza A virus guide the binding preferences of ammonium-based inhibitors"
J. Phys. Chem. B **136**:17987–17995 (2014) http://dx.doi.org/10.1021/jp506807y

23. Wu Y, Canturk B, Jo H, Ma C, Gianti E, Klein ML, Pinto LH, Lamb RA, **Fiorin G**†, Wang J, DeGrado WF.
"Flipping in the Pore: Discovery of Inhibitors that bind in different orientations to the Wild-Type versus the Amantadine-Resistant S31N Mutant of Influenza A Virus M2 Proton Channel"
J. Am. Chem. Soc. **136**(52):17987–17995 (2014) http://dx.doi.org/10.1021/ja508461m

24. Dong H, **Fiorin G**, DeGrado WF, Klein ML.
"Proton release from the histidine-cluster in the M2 channel of the influenza A virus via molecular dynamics simulations"
J. Phys. Chem. B **118**(44):12644–12651 (2014) http://dx.doi.org/10.1021/jp5102225

25. Dong H, Klein ML, **Fiorin G**.
"Counterion-assisted Cation Transport in a Biological Calcium Channel"
J. Phys. Chem. B **118**(32):9668–9676 (2014) http://dx.doi.org/10.1021/jp5059897

26. Dewan S, Carnevale V, Bankura A, Eftekhari-Bafrooei A, **Fiorin G**, Klein ML, Borguet E.
"Structure of Water at Charged Interfaces: A Molecular Dynamics Study"
Langmuir **30**(27):8056–8065 (2014) http://dx.doi.org/10.1021/la5011055

27. Bejagam KK, **Fiorin G**, Klein ML, Balasubramanian S.
"Supramolecular Polymerization of Benzene-1,3,5-tricarboxamide: A Molecular Dynamics Simulation Study"
J. Phys. Chem. B **118**(19):5218–5228 (2014) http://dx.doi.org/10.1021/jp502779z

28. Vidossich P, Loewen P, Carpena X, **Fiorin G**, Fita I, Rovira C
"Binding of the Anti-Tubercular Pro-Drug Isoniazid in the Heme Access Channel of Catalase–Peroxidase (KatG). A Combined Structural and Metadynamics Investigation"
J. Phys. Chem. B **118**(11):2924–2931 (2014) http://dx.doi.org/10.1021/jp4123425

29. **Fiorin G**†, Klein ML, Hénin J.
"Using collective variables to drive molecular dynamics simulations."
Mol. Phys. **22-23**:3345-3362 (2013) http://dx.doi.org/10.1080/00268976.2013.813594
(2nd most downloaded article of the *Mol. Phys.* website)

30. Dong H*, **Fiorin G***, DeGrado WF, Klein ML.
"Exploring histidine conformations in the M2 channel lumen of the influenza A virus via molecular simulations"
J. Phys. Chem. Letters **4**:3067-3071 (2013) http://dx.doi.org/10.1021/jz401672h

31. Dong H, **Fiorin G**, Carnevale V, Treptow W, Klein ML.
"Pore waters regulate ion permeation in a calcium release-activated calcium channel"
Proc. Natl. Acad. Sci. USA, **110**:17332-17337 (2013) http://dx.doi.org/10.1073/pnas.1316969110

32. Ma C*, **Fiorin G***, Carnevale V*, Wu Y, Wang J, Lamb RA, Klein ML, Pinto LH, DeGrado WF.
"Asp44 stabilizes the Trp41 gate of the M2 proton channel of influenza A virus"
Structure **21**:2033-2041 (2013) http://dx.doi.org/10.1016/j.str.2013.08.029

33. Wang J, Ma C, Wang J, Jo H, Canturk B, **Fiorin G**, Pinto LH, Lamb RA, Klein ML, DeGrado WF.
"Discovery of Dual Inhibitors of WT and the Amatandine-Resistant Mutant, S31N of M2 from Influenza A Virus"
J. Med. Chem. **56**(7):2804–2812 (2013). http://dx.doi.org/10.1021/jm301538e

34. Wang J, Wu Y, Ma C, **Fiorin G**, Wang J, Pinto LH, Lamb RA, Klein ML, DeGrado WF
"Structure and inhibition of the drug-resistant S31N mutant of the M2 ion channel of influenza A virus"
Proc. Natl. Acad. Sci. USA **110**(4):1315-20 (2013) http://dx.doi.org/10.1073/pnas.1216526110

35. Wang J, Ma C, **Fiorin G**, Carnevale V, Wang T, Hu F, Lamb RA, Pinto LH, Hong M, Klein ML, DeGrado WF.
"Molecular dynamics simulation directed rational design of inhibitors targeting drug-resistant mutants of influenza A virus M2."
J. Am. Chem. Soc. **133**(32):12834–41 (2011). http://dx.doi.org/10.1021/ja204969m

36. Donald JE*, Zhang Y*, **Fiorin G***, Carnevale V, Slochower DR, Gai F, Klein ML, Degrado WF.
"Transmembrane orientation and possible role of the fusogenic peptide from parainfluenza virus 5 (PIV5) in promoting fusion."
Proc Natl Acad Sci USA **108**(10):3958–63 (2011). http://dx.doi.org/10.1073/pnas.1019668108

37. Carnevale V*, **Fiorin G***, Levine BG*, DeGrado WF and Klein ML.
"Multiple Proton Confinement in the M2 Channel from the Influenza A Virus."
J. Phys. Chem. C **114**(48):20856–20863 (2010). http://dx.doi.org/10.1021/jp107431g

38. Acharya R*. Carnevale V*, **Fiorin G***, Levine BG*, Polishchuck AL*, Balannik V, Samish I, Lamb RA, Pinto LH, Klein ML, DeGrado WF.
"Structure and mechanism of proton transport through the transmembrane tetrameric M2 protein bundle of the influenza A virus."
Proc Natl Acad Sci USA **107**(34):15075-80 (2010). http://dx.doi.org/10.1073/pnas.1007071107

39. Vidossich P, **Fiorin G**, Alfonso Prieto M, Derat E, Shaik S, Rovira C.
"On the role of water in peroxidase catalysis: a theoretical investigation of HRP compound I formation."
J. Phys. Chem. B **114**(15):5161-9 (2010). http://dx.doi.org/10.1021/jp911170b

40. Balannik V, Carnevale V, **Fiorin G**, Levine BG, Lamb RA, Klein ML, DeGrado WF, Pinto LH.
"Functional studies and modeling of pore-lining residue mutants of the influenza A virus M2 ion channel."
Biochemistry **49**(4):696-708 (2010). http://dx.doi.org/10.1021/bi901799k

41. Hénin J, **Fiorin G**, Chipot C, Klein ML.
"Exploring Multidimensional Free Energy Landscapes Using Time-Dependent Biases on Collective Variables."
J. Chem. Theory Comput. **6**(1):35-47 (2010). http://dx.doi.org/10.1021/ct9004432

42. **Fiorin G**, Pastore A, Carloni P, Parrinello M.
"Using metadynamics to understand the mechanism of calmodulin/target recognition at atomic detail."
Biophys. J. **91**(8):2768-2777 (2006). http://dx.doi.org/10.1529/biophysj.106.086611

43. **Fiorin G**, Biekofsky RR, Pastore A, Carloni P.
"Unwinding the helical linker of calcium-loaded calmodulin: a molecular dynamics study."
Proteins **61**(4):829-39 (2005). (Cover article) http://dx.doi.org/10.1002/prot.20597

44. **Fiorin G**, Maglione E, Ferreira LS.
"Theoretical description of deformed proton emitters: nonadiabatic quasi-particle method."
Phys. Rev. C **67**(5):054302 (2003). http://dx.doi.org/10.1103/PhysRevC.67.054302

BOOK CHAPTERS AND COMMENTARIES

1. **Fiorin G**, Klein ML, DeVane RH, Shinoda W.
"Computer Simulation of Self-assembling Macromolecules"
Advances in Polymer Science **262**:93-107 (2013) http://dx.doi.org/10.1007/12_2013_262

2. **Fiorin G**, Carnevale V, DeGrado WF.
"The flu's proton escort."
Science **330**:456-8 (2010). http://dx.doi.org/10.1126/science.1197748

INVITED TALKS, PRESENTATIONS AND POSTERS

02/25/2023 *"Membrane free-energy landscapes derived from atomistic dynamics explain nonuniversal cholesterol-induced stiffening"*, Biophysical Society Annual Meeting (poster)

10/26/2022 "*Quantifying energy landscapes of biomembrane deformation*", Symposium "*Ions, membrane and channels: Multiscale simulations from quantum to coarse-grain. A symposium in honor of Mike Klein.*", Rome, Italy (invited talk)

6/8/2022 "*Quantifying energy landscapes of biomembrane deformation*", Biophysical Society conference on *"Molecular Biophysics of Membranes*", Tahoe City (talk)

4/28/2022 "*Potentials of mean force of biomembrane deformation*", Applied Mathematics seminar, Drexel University, Philadelphia, PA (invited talk).

9/23/2021 "*Updates and improvements in the Colvars module*", NAMD Developer Workshop (talk)

8/11/2021 "*Updates and improvements in the Colvars package*", LAMMPS Virtual Workshop and Symposium (talk)

3/16/2020 "*Comparison of mechanical properties of aramid fibers at controlled microscopic conditions*" ACS fall national meeting, Philadelphia (talk, canceled).

8/11/2019 "*Coexistence of lipid phases stabilizes interstitial water in the outer layer of mammalian skin*" Gordon Research Conference "Barrier function of mammalian skin", Waterville Valley (poster).

8/21/2018 "*Aggregation of poly(p-phenylene terephthalamide) chains: emergence of fiber defects*", ACS fall national meeting, Boston (poster).

6/11/2018 "*Collective Variables Module Updates*", NAMD developers workshop, UIUC (talk)

9/27/2017 "*Hands-on Workshop on Enhanced Sampling and Free-Energy Calculation*", UIUC (invited lecturer)

6/13/2017 "*Modeling the barrier function of mammalian skin in molecular detail*", Department of Biology, University of Fribourg, Switzerland (invited talk)

6/8/2017 "*Molecular structure of the outer lipid barrier of mammalian skin*", Workshop "*The future of biomembrane simulations: hidden pitfalls and future challenges*", Lyon, France (invited talk)

5/22/2017 "*Whole-system collective variables for free-energy calculations*", NAMD developers workshop, University of Chicago (talk)

2/28/2017 "*Accelerating MD simulations of complex lipid assemblies*", Workshop "*Frontiers in Computational Biophysics and Biochemistry*", RIKEN AICS, Kobe, Japan (invited talk)

2/8/2017 "*Predictive CG-MD simulations of lipid membrane structure: application to the skin's outer barrier*" Chemistry Department, Boston University (invited talk)

8/24/2016 "*Lipid phase coexistence forms the basis of the permeability barrier of the outer skin layer*", ACS meeting, Philadelphia (talk)

8/23/2016 "*Molecular structure of the human skin barrier and its response to external agents*", Symposium "*Polymer science for everyday things*", ACS meeting, Philadelphia (talk)

5/26/2016 "*Performance improvements in the Colvars module: towards supramolecular systems*", NAMD developer workshop, University of Chicago (invited talk)

4/13/2016 "*Tracing the geometry of water clusters to understand selectivity for drugs*", Applied Mathematics Seminar, Temple University (invited talk)

10/5/2015 "*Predicting activity and permeation of small-molecule drugs at biological membranes by molecular dynamics simulations*", University of the Sciences in Philadelphia (invited talk)

8/19/2015 "*Advanced Modeling of the Human Skin Barrier*", Gordon Research Conference on "Barrier Function of Mammalian Skin, Waterville Valley, NH (poster)

8/19/2015 "*Modeling permeation through the lipid matrix of the stratum corneum via molecular dynamics simulations*", Gordon Research Conference on "Barrier Function of Mammalian Skin, Waterville Valley, NH (poster)

5/28/2015 "*Modeling the barrier function of mammalian skin in molecular detail*" National Institute of Health, Rockville, MD (invited talk)

2/9/2015 "*Advanced Modeling of the Human Skin Barrier*" Biophysical Society National Meeting, Baltimore, MD (poster)

2/9/2015 "*Dehydration of Multilamellar Fatty Acid Membranes: Towards a Computational Model of the Stratum Corneum*" Biophysical Society National Meeting, Baltimore, MD (poster)

2/8/2015 "*New Developments in the Collective Variables Module: More Flexible, More Interactive*" Biophysical Society National Meeting, Baltimore, MD (poster)

11/14/2014 "*Confined water molecules used as a template for drug design and as a tool to study the (dis)assembly of human skin*", Dept. of Biochemistry, Rowan University (invited talk)

10/15/2014 "*Confined water molecules used as a template for drug design and as a tool to study the (dis)assembly of human skin*", Physics Colloquium, Drexel University (invited talk)

9/16/2014 "*Confined water molecules used as a template for drug design and as a tool to study the (dis)assembly of human skin*", Department of Chemistry faculty research seminar, Temple University (invited talk)

9/3/2014 "*Simulation studies of co-aggregation in the mechanism of vesicle fusion and the assembly of human skin*", Biomembrane Days Symposium, Berlin, Germany (invited talk)

8/10/2014 "*Deconstructing the pathways of ion conduction to describe the geometry of inhibition sites of the flu's proton channel*", American Chemical Society National Meeting, San Francisco, CA (poster)

8/10/2014 "*Water molecules work in concert to direct the traffic of protons in a viral channel*", American Chemical Society National Meeting, San Francisco, CA (invited talk)

4/01/2014 "*Advanced modeling of the human skin barrier*", Interdisciplinary Research Group seminar, University of Pennsylvania, Philadelphia, PA (invited talk)

2/18/2014 "*Role of model proteins in membrane fusion*", Biophysical Society National Meeting, San Francisco, CA (poster)

4/17/2013 "*Proton conduction in biological membranes*", Workshop on "Frontiers in Neutron Structural Biology", Oak Ridge National Laboratory, TN (invited talk)

8/21/2012 "*Molecular dynamics simulation-directed rational design of inhibitors targeting drug-resistant mutants of influenza A virus M2*", American Chemical Society National Meeting, Philadelphia, PA (talk)

2/29/2012	"*Mapping water density to design new blockers against a viral proton channel*", Biophysical Society Annual Meeting, San Diego, CA (poster)
10/3/2011	"*Mapping water density to design new blockers against a viral proton channel*", Workshop on "Innovative Approaches to Computational Drug Discovery", CECAM, Lausanne, Switzerland (invited talk)
3/3/2011	"*Role of the fusogenic peptide from parainfluenza virus 5 in promoting fusion*", Biophysical Society National Meeting, Baltimore, MD (poster)
2/24/2010	"*Electrostatics of water clusters in the M2 channel of the influenza A virus*", Biophysical Society National Meeting, San Francisco, CA (poster)
3/1/2009	"*Collective variable-based calculations in NAMD*", Biophysical Society National Meeting, Boston, MA (poster)
8/13/2008	"*Amplitude and time scale of large scale motions in calmodulin*", American Chemical Society Fall National Meeting, Philadelphia, PA (poster + SciMix)
6/19/2008	"*Amplitude and time scale of large scale motions in calmodulin*", International School for Advanced Studies, Trieste, Italy (invited talk)
6/8/2008	"*Amplitude and time scale of large scale motions in calmodulin*", Meeting on "Pushing the Boundaries of Biomolecular Simulations", Ascona, Switzerland (poster)
11/29/2007	"*Using metadynamics to understand the mechanism of calmodulin/target recognition at atomic detail*", University of Illinois-Urbana Champaign, IL (invited talk)
10/5/2006	"*Calmodulin dynamics and NMR properties from MD simulations*", Slovenian-Italian NMR Consortium Inaugural Symposium, Trieste, Italy (invited talk)
10/4/2005	"*Calmodulin: dynamics and target recognition by molecular dynamics simulations*" Bunsen International discussion meeting, Tuzting - Munich, Germany (invited talk)
8/15/2005	"*Calmodulin: dynamics and target recognition by molecular dynamics simulations*" School on Computer Simulations in Condensed Matter, Erice, Italy (poster)
4/25/2005	"*Calmodulin: dynamics and target recognition by molecular dynamics simulations*" Swiss-Italian University, Lugano, Switzerland (invited talk)

SYNERGISTIC ACTIVITIES AND OUTREACH

2008 – ongoing	Lead developer of the collective variables software module (*Colvars*) for enhanced sampling and free-energy calculations (https://colvars.github.io/).
2008 – ongoing	Technical support of trainees via the forums of the GROMACS, LAMMPS, NAMD, and VMD software packages.
2007 – ongoing	Reviewer for scientific journals: *ACS Central Science, ACS Nano, Biomacromolecules, Biophys J, Chem Sci, Comp Mater Sci, Comp Phys Comm, Frontiers Mol Biosci, JACS, JCIM, JCTC, J Phys Chem B, J Phys Chem Lett, Langmuir, Macromolecules, PLOS Comp Biol, PLOS One, PNAS, Sci Rep, Soft Matter*
2014 – ongoing	Member of the American Association for the Advancement of Sciences (AAAS)
2007 – ongoing	Member of the Biophysical Society
2022, 2023	Judge, Postbac Poster Day (NIH intramural program)
2022, 2023	Judge, Fellows Award for Research Excellence (NIH intramural program)

2016 – 2020	Co-advised with Benjamin Seibold PhD candidate Joshua Finkelstein, Applied Mathematics program, Temple University (defense date: 6/5/20); currently at Los Alamos National Labs.
2013 – 2019	Co-supervised with Michael Klein the following postdoctoral researchers at Temple: Hao Dong (later at: Nanjing Univ), Hemant Kashyap (later at: IIT Delhi), Eleonora Gianti (later at: Swarthmore College), Christopher MacDermaid (later at: GlaxoSmithKline), Santosh Mogurampelly (later at: IIT Jodhpur).
2015 – 2019	Editorial Board Member, *Scientific Reports*; resigned in 2019.
2011 – 2015	Instructor in Biostatistics for undergraduate and programs in biology, biomedical engineering, pharmacy and health professions, Temple University
2010 – 2013	Adjunct Instructor in Statistical Thermodynamics, chemistry program, Temple University
11/2/2015	External committee member, PhD thesis defense, Asghar Razavi (moved to: Weill Cornell Medical College, NY), Chemistry department, Temple University
7/9 – 7/13/2018	Organizer, Workshop "*Modeling supra-molecular structures with LAMMPS*", Temple University, Philadelphia, PA
2008 – 2019	Member of the American Chemical Society
6/1 – 6/2/2019	Organizer, Workshop "*Current trends in molecular dynamics software design*", Temple University, Philadelphia, PA
8/15 – 8/18/2016	Organizer, Workshop "*Molecular dynamics of modern materials with LAMMPS*", August 15-18, Temple University (60 registered participants), and Symposium "*Molecular dynamics of materials from assembly to fracture*" (100 registered participants)
2015 – 2016	Undergraduate research mentor for the *Science Scholars* program (Abyaad Kashem, Biophysics program, class of 2018)
8/23/2016	Lecturer, Symposium "*Polymer science for everyday things*", ACS meeting, Philadelphia. 40 high school teachers participated in the symposium.
7/6 – 7/10/2015	Instructor and co-organizer, School on *"Molecular Dynamics for Biomolecules and Nanomaterials*", Temple University
1/30/2015	Interview with KYW News Radio on the discovery of new anti-influenza drugs
10/16/2014	Guest lecturer, Physics Colloquium (undergraduate program), Drexel University
8/18 – 8/22/2014	Instructor, School on *"Molecular Dynamics for Biomolecules and Nanomaterials*", Temple University
3/18/2014	Guest lecturer, course on "*Free Energy Calculations*", City University of New York, chemistry and biology PhD programs
4/16 – 4/18/2013	Invited speaker and panelist, Workshop on "Frontiers in Neutron Structural Biology", Oak Ridge National Laboratory, TN
2/24 – 3/10/2013	Visiting instructor, course on "*Free Energy Calculations and Advanced Molecular Dynamics Simulations*", Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore, India
4/2012	Guest lecturer on "*Experimental determination of protein structure*", course on "*Introduction to Structural Bioinformatics*", Chemistry and Biology PhD programs, Temple University

10/2009	Guest lecturer, course in "*Physical chemistry II*", Chemistry BA and BS programs, Temple University
6/11 – 6/15/2007	Lecturer, workshop on "*High Performance Computing*", School of Arts and Sciences and School of Engineering, University of Pennsylvania
11/21/2005	Guest lecturer, United World College of the Adriatic (high school), Duino, Italy

ADMINISTRATION AND RESEARCH SUPPORT

3/2018 – ongoing	Administrator of scientific computing systems for the Computational Structural Biology and Theoretical Molecular Biophysics laboratories, National Institutes of Health.
9/2016 – ongoing	Administrator of scientific data storage/transfer systems, ICMS, Temple University (volunteer-only effort since 2020).
10/2016 – 9/2018	Proposal preparation and supervision of computational material science sub-projects in the US Army Research Lab contract W911NF-16-2-0189 "Advanced Ballistics Technology: Material Development, Characterization and Computational Modeling."
7/2011 – 12/2018	Supercomputing allocations manager for the Institute for Computational Molecular Science, Temple University (NSF-XSEDE, DOE-INCITE and DOE-ERCAP programs)
1/2018 – 12/2018	Co-PI with Benoit Roux and Christophe Chipot of the allocation "*The Free Energy Landscapes Governing Membrane Protein Function*", DOE-INCITE supercomputing program – 92,300,000 core-hours
8/11/2017	Panel reviewer, National Academy Committee on Molecular Dynamics Simulations, Washington, DC
4/6 – 4/7/2016	Panel reviewer, Advanced Scientific Computing Research Leadership Computing Challenge (ALCC), Department of Energy, Rockville, MD
5/2016 – 4/2018	Co-PI with Vincenzo Carnevale, Michael Klein and Christopher MacDermaid of the allocation "*Ion channels response in physiological conditions: toward a computational framework for nociception*", NSF-Blue Waters supercomputing program – 11,400,000 node-hours
1/2015 – 12/2015	Co-PI with Michael Klein and Russell DeVane of the allocation "*Shutdown and recovery of the barrier function of human skin*", DOE-INCITE supercomputing program – 92,000,000 core-hours
1/2014 – 12/2014	Co-PI with Michael Klein and Russell DeVane of the allocation "*Assembling and sustaining the acid mantle of the human skin barrier*", DOE-INCITE supercomputing program – 75,000,000 core-hours
7/2012 – 7/2015	Co-PI with Michael Klein and Axel Kohlmeyer of the NSF grant 1212416 "*Building Computational Models to Probe Membrane Fusion*" – $405,999
12/2013	Reviewer of funding proposals for the Human Brain Project, European Union
1/2013 – 12/2013	Co-PI with Michael Klein and Russell DeVane on the project "*Advanced modeling of the human skin barrier*", DOE-INCITE supercomputing program – 65,000,000 core-hours
1/2011 – 12/2012	Co-PI with Michael Klein, Russell DeVane, Vincenzo Carnevale and Axel Kohlmeyer of the project CHM045 "*Coarse grained molecular dynamics studies of vesicle formation*

and fusion" under the DOE INCITE supercomputing program – 48,000,000 core-hours over 2 years on OLCF Jaguar