Giacomo Fiorin – Curriculum Vitae

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Google Scholar: http://goo.gl/Q3TBQU

ACADEMIC APPOINTMENTS

07/2015 – present	Associate Professor of Research, Temple University
01/2017 – present	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)

CURRENT RESEARCH INTERESTS

- Structure and mechanics of biological membranes.
- Development of high-performance molecular dynamics simulation software.
- Molecular structure of the stratum corneum of human skin and permeation of small molecules.
- Structure of self-assembled polymer fibers for high-performance materials.
- Mechanisms of membrane fusion in eukaryotes and in viruses.
- Development of coarse-grained force fields for biomembrane lipids and embedded proteins.
- Optimization of numerical integration schemes for coarse-grained MD simulations.

PEER-REVIEWED PUBLICATIONS

In reverse chronological order; asterisks indicate equal contributions.

1. MacDermaid CM, DeVane RH, Klauda JB, Klein ML, **Fiorin G**.
   "High-resolution model of lamellar phase coexistence in the lipid matrix of stratum corneum."
   (*in preparation*)
2. 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
3. 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
4. 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
5. 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
6. 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
7. 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
8. 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
9. 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
10. 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

11. 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

12. 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

13. 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

14. 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

15. **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
(most downloaded article of the *Mol. Phys.* website)

16. 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

17. **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

18. 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

19. 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

20. 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

21. 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

22. 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

23. 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

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

25. 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

26. 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

27. 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

28. 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

29. 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

30. **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

31. **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

32. **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

INVITED TALKS, PRESENTATIONS AND POSTERS

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

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

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

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

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

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

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

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)

09/16/2014 "*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)

09/03/2014 "*Simulation studies of co-aggregation in the mechanism of vesicle fusion and the assembly of human skin*", Biomembrane Days Symposium, Berlin, Germany (invited talk)

08/10/2014 "*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)

08/10/2014 "*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)

04/01/2014 "*Advanced modeling of the human skin barrier*", Interdisciplinary Research Group seminar, University of Pennsylvania, Philadelphia, PA (invited talk)

02/18/2014 "*Role of model proteins in membrane fusion*", Biophysical Society National Meeting, San Francisco, CA (poster)

04/17/2013 "*Proton conduction in biological membranes*", Workshop on "Frontiers in Neutron Structural Biology", Oak Ridge National Laboratory, TN (invited talk)

08/21/2012 "*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)

02/29/2012 "*Mapping water density to design new blockers against a viral proton channel*", Biophysical Society Annual Meeting, San Diego, CA (poster)

10/03/2011 "*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)

03/03/2011 "*Role of the fusogenic peptide from parainfluenza virus 5 in promoting fusion*", Biophysical Society National Meeting, Baltimore, MD (poster)

02/24/2010 "*electrostatics of water clusters in the M2 channel of the influenza A virus*", Biophysical Society National Meeting, San Francisco, CA (poster)

03/01/2009 "*Collective variable-based calculations in NAMD*", Biophysical Society National Meeting, Boston, MA (poster)

08/13/2008 "*Amplitude and time scale of large scale motions in calmodulin*", American Chemical Society Fall National Meeting, Philadelphia, PA (poster + SciMix)

06/19/2008 "*Amplitude and time scale of large scale motions in calmodulin*", International School for Advanced Studies, Trieste, Italy (invited talk)

06/08/2008 "*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)

10/05/2006 "*Calmodulin dynamics and NMR properties from MD simulations*",
Slovenian-Italian NMR Consortium Inaugural Symposium, Trieste, Italy (invited talk)

10/04/2005 "*Calmodulin: dynamics and target recognition by molecular dynamics simulations*"
Bunsen International discussion meeting, Tuzting - Munich, Germany (invited talk)

08/15/2005 "*Calmodulin: dynamics and target recognition by molecular dynamics simulations*"
School on Computer Simulations in Condensed Matter, Erice, Italy (poster)

04/25/2005 "*Calmodulin: dynamics and target recognition by molecular dynamics simulations*"
Swiss-Italian University, Lugano, Switzerland (invited talk)

SYNERGISTIC ACTIVITIES AND OUTREACH

2008 – ongoing Developer of the collective variables (*Colvars*) module (http://colvars.github.io/) with collaborators Jérôme Hénin (CNRS, Paris, France), Axel Kohlmeyer (Temple)

2014 – ongoing Member of the American Association for the Advancement of Sciences (AAAS)

2008 – ongoing	Reviewer for the journals: *JACS, PNAS, JCTC, J Phys Chem B, J Phys Chem Lett, Comp Phys Comm, Biophys J, Langmuir, PLOS Comp Biol, PLOS One, Scientific Reports, ACS Nano, Soft Matter, Computational Materials Science*
2015 – ongoing	Editorial Board Member, *Scientific Reports*
2016 – ongoing	Co-advisor with Benjamin Seibold of PhD candidate Joshua Finkelstein, Applied Mathematics program, Temple University
2008 – ongoing	User support on the NAMD, LAMMPS and VMD software mailing lists
2015 – ongoing	Mentor of undergraduate researchers for the *Science Scholars* program (Abyaad Kashem, Biophysics program, class of 2018)
2017/06/1-2	Organizer, Workshop "*Current trends in molecular dynamics software design*", Temple University, Philadelphia, PA
2016/8/15-18	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)
2016/8/23	Lecturer, Symposium "*Polymer science for everyday things*", ACS meeting, Philadelphia. 40 high school teachers participated in the symposium.
2016 – ongoing	Member, Temple Materials Institute (TMI)
2015/04/6-7	Panel reviewer for the Advanced Scientific Computing Research call, Department of Energy, Rockville, MD
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
03/18/2014	Guest lecturer, course on "*Free Energy Calculations*", City University of New York, chemistry and biology PhD programs
12/2013	Reviewer of proposals for the Human Brain Project competitive call, European Union
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
04/2012	Guest lecturer on "*Experimental determination of protein structure*", course on "*Introduction to Structural Bioinformatics*", Chemistry and Biology PhD programs, Temple University
2012 – ongoing	Member of the American Chemical Society (ACS)
10/2009	Guest lecturer, course in "*Physical chemistry II*", Chemistry BA and BS programs, Temple University
2007 – ongoing	Member of the Biophysical Society

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

05/2016 – 04/2018 Co-PI with Vincenzo Carnevale, Michael Klein and Christopher MacDermaid of the project "*Ion channels response in physiological conditions: toward a computational framework for nociception*", NSF-Blue Waters supercomputing program – 11,400,000 node-hours

01/2015 – 12/2015 Co-PI with Michael Klein and Russell DeVane of the project "*Shutdown and recovery of the barrier function of human skin*", DOE-INCITE supercomputing program – 92,000,000 core-hours

01/2014 – 12/2014 Co-PI with Michael Klein and Russell DeVane of the project "*Assembling and sustaining the acid mantle of the human skin barrier*", DOE-INCITE supercomputing program – 75,000,000 core-hours

07/2012 – present Co-PI with Michael Klein and Axel Kohlmeyer of the NSF grant 1212416 "*Building Computational Models to Probe Membrane Fusion*" – $405,999 (2012 – 2015)

01/2013 – 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

01/2011 – 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

07/2011 – present Supercomputing allocations manager for ICMS (NSF-XSEDE, DOE-INCITE and DOE-ERCAP programs)