

Giacomo Fiorin - CV

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Appointments

07/2011 – present Assistant Professor of Research
College of Science and Technology and Institute for Computational Molecular Science (ICMS), Temple University

09/2009 – 06/2011 Postdoctoral Research Associate
Institute for Computational Molecular Science (ICMS), Temple University
Postdoctoral advisor: Michael L. Klein (michael.klein@temple.edu)

05/2007 – 08/2009 Postdoctoral Research Associate
Center for Molecular Modeling (CMM), University of Pennsylvania
Postdoctoral advisor: Michael L. Klein

Education

10/2002 – 12/2006 PhD in Statistical and Biological Physics
SISSA - International School for Advanced Studies, Trieste, Italy
Thesis advisor: Paolo Carloni

10/1997 – 02/2002 Combined BS+MS (“Laurea”) in Physics
University of Padua, Italy
Thesis advisor: Enrico Maglione

Research

Design of algorithms to simulate complex macromolecular interactions; development of the collective variables module (colvars) for enhanced sampling calculations (<http://colvars.github.io/>).

Structure and dynamics of biological membranes; mechanism of membrane fusion in eukaryotes and in viruses; structure of the stratum corneum of the human skin and permeation of chemicals; development of coarse-grained force fields for membrane lipids and embedded proteins.

Mechanism of proton conduction through the M2 viral channel of the influenza A virus: modeling the hydration of drug-binding sites to guide the design of new inhibitors; prediction of fitness for potential mutants; development of novel computational screening methods.

Peer-reviewed publications

In reverse chronological order; asterisks, when present, indicate equal contributions.

1. Dong H, **Fiorin G**, Klein ML.
“Counterion-assisted Cation Transport in a Biological Calcium Channel”
(under review)
2. Kumar BK, **Fiorin G**, Klein ML, Balasubramanian S.
“Supramolecular Polymerization of Benzene-1,3,5-tricarboxamide: A Molecular Dynamics Simulation Study”
(under review)
3. 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, in press (2014)
4. **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)
5. 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>
6. **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
7. 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>
8. 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>
9. 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 Amantadine-Resistant Mutant, S31N of M2 from Influenza A Virus”
J. Med. Chem. **56**(7):2804–2812 (2013). <http://dx.doi.org/10.1021/jm301538e>
10. 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>
11. 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>

12. 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>
13. **Fiorin G**, Carnevale V, DeGrado WF.
 “The flu's proton escort.” (comment on Science 330:505-508 and Science 330:509-512)
Science **330**:456-8 (2010). <http://dx.doi.org/10.1126/science.1197748>
14. 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>
15. 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>
16. 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>
17. 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>
18. 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>
19. **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>
20. **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>
21. **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>

Teaching, synergistic activities and outreach

2011 – present	Primary instructor Biostatistics course (3 credits) Biology (BA, BS, MS and PhD programs), bioengineering (BS program) Temple University
2010 – present	Teaching Assistant Statistical thermodynamics Chemistry (PhD program), Temple University
2008 – present	Reviewer for scientific journals: <i>PNAS</i> , <i>Plos Comp Biol</i> , <i>J Phys Chem B</i> , <i>Comp Phys Comm</i> , <i>Biophys J</i> , <i>Scientific Reports</i>
2008 – present	User support on the NAMD, LAMMPS and VMD mailing lists
2007 – present	Member, Biophysical Society
2012	Guest lecture on “ <i>Experimental determination of protein structures</i> ” Introduction to Structural Bioinformatics, Chemistry and Biology (PhD programs), Temple University
2009	Guest lecture Physical chemistry II Chemistry (BA and BS programs), Temple University
2007	Lecturer at the High Performance Computing workshop University of Pennsylvania

Grants, administration and research support

07/2011 – present	Supercomputing allocations manager for ICMS (NSF-XSEDE, DOE-INCITE and DOE-ERCAP programs)
01/2014 – present	Co-PI with Michael Klein (PI) and Russell DeVane on the project “ <i>Assembling and sustaining the acid mantle of the human skin barrier</i> ” under the DOE INCITE supercomputing program – 75,000,000 core-hours on OLCF Titan
07/2012 – present	Co-PI with Michael Klein (PI) and Axel Kohlmeyer of the NSF grant 1212416 “ <i>Building Computational Models to Probe Membrane Fusion</i> ” – \$405,999 award (3 years)
01/2013 – 12/2013	Co-PI with Michael Klein (PI) and Russell DeVane on the project “ <i>Advanced modeling of the human skin barrier</i> ” under the DOE INCITE supercomputing program – 65,000,000 core-hours on OLCF Titan (project mentioned in National Geographic Daily News – 11/12/12)
01/2011 – 12/2012	Co-PI with Michael Klein (PI), Russell DeVane, Vincenzo Carnevale and Axel Kohlmeyer of the project CHM045 “ <i>Coarse grained molecular dynamics studies of vesicle formation and fusion</i> ” under the DOE INCITE supercomputing program – 48,000,000 core-hours over 2 years on OLCF Jaguar