

Curriculum Vitae

Feng Ding

Department of Biochemistry and Biophysics
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Education

- Ph.D., 2004 — Physics; Boston University; Boston, MA, USA
- M.A., 2001 — Physics; Boston University; Boston, MA, USA
- B.S. honors, 1997— Physics; Nanjing University; Nanjing, Jiangsu, China

Professional Experience

- 2008-present: Research Assistant Professor, Department of Biochemistry and Biophysics, University of North Carolina at Chapel Hill
- 2006-2008: Research Associate, Department of Biochemistry and Biophysics, University of North Carolina at Chapel Hill
- 2004-2006: Postdoctoral Fellow, Department of Biochemistry and Biophysics, University of North Carolina at Chapel Hill
- 2001-2004: Research Assistant, Department of Physics, Boston University
- 1999-2001: Teaching Assistant, Department of Physics, Boston University
- 1997-1999: Teaching Assistant, Department of Physics, Nanjing University

Honors, Awards

- 2005: Postdoctoral Award for Research Excellence, University of North Carolina at Chapel Hill
- 1997: Excellent Graduate, Nanjing University, 1997
- 1993-1997: Recipient of People's Stipend, Nanjing University

Bibliography

A. Original research (ISI Web of Science citations > 1000; H-index: 24)

Molecular recognition

1. O. Dagliyan, K. D'Auria, **F. Ding***, Nikolay V. Dokholyan*, "Ab initio prediction of protein-peptide interactions using molecular dynamics simulations", *Structure*, *in press* (2011)
2. **F. Ding**, S. Yin, and N. V. Dokholyan, "Rapid flexible docking using a stochastic rotamer library of ligands" *J. Chem. Info. Model.* **50**(9):1623-32 (2010)

Protein engineering and protein design

3. A. Karginov, **F. Ding**, N. V. Dokholyan, and K. M. Hahn, "Engineered allosteric regulation of kinases in living cells" *Nature Biotechnology*, **28** (7) (2010)
4. M. P. Torres, M. J. Lee, **F. Ding**, C. Purbeck, B. Kuhlman, N. V. Dokholyan, and H. G. Dohlman, "G protein mono-ubiquitination by the Rsp5 ubiquitin ligase" *Journal of Biological Chemistry*, **284**: 8940-8950 (2009)
5. S. Yin, **F. Ding**, and N. V. Dokholyan, "Modeling backbone flexibility improves protein stability estimation" *Structure*, **15**: 1567-1576 (2007)
6. S. Yin, **F. Ding**, and N. V. Dokholyan, "Eris: An automated estimator of protein stability" *Nature Methods*, **4**: 466-467 (2007)
7. **F. Ding** and N. V. Dokholyan, "Emergence of protein fold families through rational design" *Public Library of Science Computational Biology*, **2**: e85 (2006)
8. V. V. Demidov, N. V. Dokholyan, C. Witte-Hoffman, P. Chalasani, H.-W. Yiu, **F. Ding**, Y. Yu, C. R. Cantor, N. E. Broude, "Fast complementation of split fluorescent protein triggered by DNA hybridization". *Proceedings of the National Academy of Sciences USA*, **103**: 2052-2056 (2006)

GPCR modeling

9. Diatchenko, L., **Ding, F.**, Dokholyan, N. V., Gauthier, J., Gold, M., and Maixner, W., "Mu opioid receptor 6-transmembrane isoforms: potential therapeutic target for new effect opioids", *British Journal of Pharmacology*, *in press* (2011)
10. A.W.R. Serohijos, S. Yin, **F. Ding**, J. Gauthier, D.G. Gibson, V. Setola, W. Maixner, N.V. Dokholyan, and L. Diatchenko, "Structural basis for MOR1 binding and activation" *Structure*, *in press* (2011)

Protein folding, conformation dynamics, stability, and functions

11. P. Kota*, **F. Ding***, S. Ramachandran*, and N. V. Dokholyan, "Gaia: Automated quality assessment of protein structure models", *Bioinformatics*, **27**:2209-2215 (2011)
12. B. A. Kesner, **F. Ding**, B. S. Temple, and N. V. Dokholyan, "N-terminal strands of filamin Ig domains act as a conformational switch under biological forces" *Proteins: Structure, Function, and Bioinformatics*, **78**: 12-24 (2010)

13. S. Ramachandran, P. Kota, **F. Ding**, and N. V. Dokholyan, "Automated minimization of steric clashes in protein structures" *Proteins: Structure, Function and Bioinformatics*, **79**:261-270 (2010)
14. D. G. Teotico, **F. Ding**, N. V. Dokholyan, B. Temple, and M. R. Redinbo, "Active nuclear receptors exhibit highly correlated AF-2 domain motions" *Public Library of Science Computational Biology* **4**: e1000111(2008)
15. **F. Ding**, D. Tsao, H. Nie, N.V. Dokholyan "Ab initio folding of proteins using all-atom discrete molecular dynamics" *structure* **16**: 1010-1018 (2008)
16. Y. Chen, **F. Ding**, H. Nie, A. W. Serohijos, S. Sharma, K. C. Wilcox, S. Yin, and N. V. Dokholyan, "Protein folding: then and now" *Archives of Biochemistry and Biophysics*, **469**: 4-19 (2008)
17. R. Lam, J. M. Borreguero, **F. Ding**, N. V. Dokholyan, S. V. Buldyrev, E. I. Shakhnovich, H. E. Stanley, "Parallel folding pathways in the Src SH3 domain" *Journal of Molecular Biology*, **373**: 1348-1360 (2007)
18. Y. Chen, **F. Ding**, and N. V. Dokholyan, "Fidelity of protein structure reconstruction from inter-residue proximity constraints" *Journal of Physical Chemistry B*, **111**: 7432-7438 (2007)
19. S. Sharma, **F. Ding**, and N. V. Dokholyan, "Multi-scale modeling of nucleosome dynamics" *Biophysical Journal*, **92**:1457-1470 (2007)
20. S. Sharma, **F. Ding**, H. Nie, D. Watson, A. Unnithan, J. Lopp, D. Pozefsky, and N. V. Dokholyan, "iFold: A platform for interactive folding simulations of proteins" *Bioinformatics*, **22**: 2693-2694 (2006)
21. A. W. Serohijos, Y. Chen, **F. Ding**, T. C. Elston, and N. V. Dokholyan, "A new structural model reveals energy transduction in dynein" *Proceedings of the National Academy of Sciences USA*, **103**: 18540-18545 (2006)
22. **F. Ding**, W. Guo, N.V. Dokholyan, E.I. Shakhnovich, and J.-E. Shea, "Reconstruction of the src-SH3 protein domain transition state ensemble using multiscale molecular dynamics simulations", *Journal of Molecular Biology* **350**:1035-1050 (2005)
23. **F. Ding** and N.V. Dokholyan, "Simple but predictive protein models", *Trends in Biotechnology* **23**:450-455 (2005)
24. **F. Ding**, R.K. Jha, and N.V. Dokholyan, "Scaling behavior and structure of denatured proteins", *Structure* **13**:1047-1054 (2005)
25. **F. Ding***, S.V. Buldyrev, and N.V. Dokholyan, "Folding Trp-cage to NMR resolution native structure using a coarse-grained protein model", *Biophysical Journal* **88**: 147-155 (2005)
26. R.D.S. Dixon, Y. Chen, **F. Ding**, S.D. Khare, K.C. Prutzman, M.D. Schaller, S.L. Campbell, and N.V. Dokholyan, "New insights into FAK signaling and localization based on detection of a FAT domain folding intermediate", *Structure* **12**: 2161-2171 (2004)
27. J.M. Borreguero, **F. Ding**, S.V. Buldyrev, H.E. Stanley and N.V. Dokholyan, "Multiple Folding

Pathways of the SH3 domain”, *Biophysical Journal* **87**: 521-533 (2004)

28. N.V. Dokholyan, L. Li, **F. Ding** and E.I. Shakhnovich, “Topological determinants of protein folding”. *Proceedings of National Academy of USA* **99**: 8637-8641 (2002)
29. **F. Ding***, N.V. Dokholyan, S.V. Buldyrev, H.E. Stanley and E.I. Shakhnovich, “Direct molecular dynamics observation of protein folding transition state ensemble”, *Biophysical Journal* **86**: 3525-3532 (2002)

RNA folding

30. **F. Ding**, C. Lavender, K.M. Weeks, and N.V. Dokholyan, “Three-Dimensional RNA Structure Determination by Hydroxyl Radical Probing”, *Pending with revision* (2011)
31. D.I. Cole, **F. Ding**, N.V. Dokholyan, and M.B. Jarstfer, “A three-dimensional model of tetrahymena telomerase RNA in the minimal telomerase complex”, *submitted* (2011)
32. C. Lavender, **F. Ding**, N. V. Dokholyan, and K. M. Weeks, “Robust and generic RNA modeling using inferred constraints: A structure for the hepatitis C virus IRES pseudoknot domain” *Biochemistry*, **49**: 4931-3. (2010)
33. C. Hajdin, **F. Ding**, N. V. Dokholyan, and K. M. Weeks, “On the significant of an RNA tertiary structure prediction.” *RNA*, **16**: 1340-9 (2010)
34. C. M. Gherghe, C. W. Leonard, **F. Ding**, N. V. Dokholyan, and K. M. Weeks, “Native-like RNA tertiary structures using a sequence-encoded cleavage agent and refinement by discrete molecular dynamics” *Journal of the American Chemical Society*, **131** 2541–2546 (2009)
35. S. Sharma, **F. Ding**, and N.V. Dokholyan, "iFoldRNA: Three-dimensional RNA structure prediction and folding", *Bioinformatics*, 24:1951-1952, (2008)
36. **F. Ding**, S. Sharma, P. Chalasani, V. V. Demidov, N. E. Broude, N. V. Dokholyan, “Large Scale Simulations of 3D RNA folding by Discrete Molecular Dynamics: From Structure Prediction to Folding Mechanisms” *RNA*, **14**: 1164-1173 (2007)

Protein misfolding and aggregation.

37. **F. Ding**, Y. Furukawa, N. Nukina, and N.V. Dokholyan, “Local unfolding of Cu, Zn Superoxide Dismutase monomer determines the morphology of fibrillar aggregates”, *Pending with revision* (2011)
38. E. A. Proctor, **F. Ding**, and N. V. Dokholyan, “Structural and thermodynamic effects of post-translational modifications in mutant and wild type Cu, Zn Superoxide Dismutase” *J. Mol. Biol.* **408**:555-567 (2011)
39. V. V. Lakhani, **F. Ding** and N. V. Dokholyan, “Poly-glutamine induced misfolding of huntingtin exon1 is modulated by the flanking sequences”, *PLoS Comput. Biol.*, **6**:e1000772 (2010)
40. **F. Ding** and N. V. Dokholyan, “Dynamical roles of metal ions and the disulfide bond in Cu, Zn superoxide dismutase folding and aggregation” *Proceedings of the National Academy of Sciences USA*, **105**: 19696-19701 (2008)
41. S. Barton, R. Jacak, S. D. Khare, **F. Ding***, and N. V. Dokholyan*, “A generalized mechanism

for polyglutamine-mediated protein aggregation" *Journal of Biological Chemistry*, **282**: 25487-25492 (2007)

42. S. Sharma, **F. Ding**, and N. V. Dokholyan, "Probing protein aggregation using simplified models and discrete molecular dynamics" *Frontiers in Bioscience*, **13**: 4795-4808 (2007)
43. **F. Ding**, K.C. Prutzman, S.L. Campbell, and N.V. Dokholyan, "Topological determinants of protein domain swapping", *Structure*, **14**:5-14 (2006)
44. S.D. Khare, **F. Ding**, K.N. Gwanmesia, and N.V. Dokholyan, "Molecular origin of polyglutamine-mediated protein aggregation in neurodegenerative diseases", *PLoS Computational Biology* **1**:230-235 (2005)
45. **F. Ding**, J. J. LaRocque, and N. V. Dokholyan, "Direct observation of protein folding, aggregation, and a prion-like conformational conversion", *Journal of Biological Chemistry* **280**: 40235-40240 (2005)
46. 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", *Physical Review E* **69**: 041908 (2004)
47. 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-beta dimer formation", *Biophysical Journal* **87**: 2310-2321 (2004)
48. S.D. Khare, **F. Ding** and N.V. Dokholyan, "Folding of Cu, Zn superoxide dismutase and Familial Amyotrophic Lateral Sclerosis", *Journal of Molecular Biology* **334**: 515-525 (2003)
49. **F. Ding***, J.M. Borreguero, S.V. Buldyrev, H.E. Stanley and N.V. Dokholyan, "A mechanism for alpha-helix to beta-hairpin transition", *Proteins: Structure, Function and Genetics* **53**: 220-228 (2003)
50. **F. Ding***, N.V. Dokholyan, S.V. Buldyrev, H.E. Stanley and E.I. Shakhnovich, "Molecular dynamics simulation of C-Src SH3 aggregation suggests a generic amyloidogenesis mechanism". *Journal of Molecular Biology* **324**:851-857 (2002)

Condensed matter physics

51. X.Y. Lei, H. Li, **F. Ding**, W.Y. Zhang, and N.B. Ming, "Novel application of a perturbed photonic crystal: High-quality filter". *Applied Physics Letter* **71**: 2889-2891 (1997)

B. Books and Chapters

1. **F. Ding**, and N. V. Dokholyan, "Discrete Molecular Dynamics Simulations of Biomolecules", in "Computational Modeling of Biological Systems: From Molecules to Pathways" Editors N. V. Dokholyan. Springer. *In Press* (2011)
2. **F. Ding**, and N. V. Dokholyan, "Multiscale modeling of RNA structure and dynamics." in "RNA 3D Structure Analysis and Prediction" Editors: N. Leontis and E. Westhof. Series "Nucleic Acids and Molecular Biology" (Series Editor: J. Bujnicki). Springer. *In press* (2011)
3. E. A. Proctor, **F. Ding**, and N. V. Dokholyan, "Discrete Molecular Dynamics." in Wiley

Interdisciplinary Reviews: Computational Molecular Science. (2010)

4. S. Yin, **F. Ding**, and N. V. Dokholyan, “Modeling mutations in proteins using Medusa and discrete molecule dynamics.” in “Protein Structure Prediction: Method and Algorithms” Editors: H. Rangwala and G. Karypis. Wiley (2010)
5. S. Yin, **F. Ding**, and N. V. Dokholyan, “Computational evaluation of protein stability change upon mutations using Eris.” in “*In Vitro Mutagenesis Protocols*” Editor: J. Braman. Humana Press (2009)
6. N.V. Dokholyan, J.M. Borreguero, S.V. Buldyrev, **F. Ding**, H.E. Stanley and E.I. Shakhnovich, “Identifying the importance of amino acids for protein folding from crystal structures”, *Methods in Enzymology* **374**: 618-640 (2003)

C. Presentations

- 2011 78th Annual Meeting of the Southeastern Section of APS, Roanoke, VA (Invited talk)
- 2011 Biochemistry and Biophysics Department Retreat, UNC (Invited talk)
- 2011 HES70 — Horizons in Emergence and Scaling, Boston (Poster)
- 2010 UNC Bioinformatics & Computational Biology Colloquium (Invited talk)
- 2010 1st Prague Protein’s Spring, Czech Republic (Invited talk)
- 2009 Invited Seminar at the Center for Neurosensory Disorders, UNC (Invited talk)
- 2009 2009 NCTS June Workshop on Critical Phenomena and Complex Systems, Taipai (Invited Talk)
- 2009 2009 Mesilla Chemistry Workshop, Mesilla, NM, USA (Invited talk)
- 2009 Biomolecular Engineering, Society of Biological Engineering’s 2nd International Conference, Santa Barbara, California, USA (Invited talk)
- 2007 RNA Structure and Function, International RNA Symposium of RNA society of North Carolina, Chapel Hill, NC, USA (Poster)
- 2006 Physics and Computation on Protein Structure, The Sixth Biannual Triangle Biophysics Symposium, Chapel Hill, NC, USA (Poster)
- 2006 DARPA Protein Conformational Design Initiation, Arlington, VA, USA (Poster)
- 2005 Protein Society Annual Meeting, Boston, MA, USA (Poster)
- 2005 eCheminfo conference, “Protein folding, Misfolding & Aggregation: Application to Disease”, Philadelphia, PA, USA (Invited talk)
- 2003 Gordon Research Conference, New Hampshire, USA (Poster)

- 2003 Boston University Science Day (Poster)
- 2002 Physics and Computation on Protein Structure, The Fourth Biannual Triangle Biophysics Symposium, Chapel Hill, NC, USA (Poster)
- 2001 Statphys XXI, Cancun, Mexico (Poster)

Teaching Record

A. Classroom teaching

- 2011 Lecture of “Introduction to protein structure and functions” for the Biophysics Society Summer School 2011, UNC
- 2008-Present Lecture of “Computational RNA Structure Determination” for the RNA biology class by Dr. Howard M. Fried
- 2006 Lecture of “Discrete Molecular Dynamics” for the Computational Biology class by Dr. Jan Hermans
- 1999-2001 Teaching Assistant for a number of beginning and advanced undergraduate courses, Boston University
- 1997-1999 Teaching Assistant for the college physics, Nanjing University

B. Rotation graduate students trained

- 2010 Onur Dagliyan — *Rotation resulted into a research paper*
- 2009 Vinal Lakhani — *Rotation resulted into a research paper*
- 2008 Sai Phanindra
- 2007 Pradeep Kota
- 2006 Daud Cole
- 2005 Ron Jacak — *Rotation resulted into a research paper*
- 2004 Ramesh K. Jha — *Rotation resulted into a research paper*

C. Summer/Rotation undergrad students trained

- 2011 Mahmoud Shobair
- 2010 Kalada Kienka (The Summer Research Experience for Undergraduates (SURE-REU) Program in Molecular Biosciences)
- 2009 Regis A. James

- 2008-2009 Kevin D'Auria — *Rotation resulted into a research paper*
- 2006-2008 Vinal Lakhani — *Rotation resulted into a research paper*
- 2006 Sunjay Barton (Partnership for Minority Advancement in the Biomolecular Sciences fellow) — *Rotation resulted into a research paper*
- 2004-2006 Joshua J. Larocque — *Rotation resulted into a research paper*
- 2004 Kenneth Nteh Gwanmesia (Summer Pre-Graduate Research Experience fellow) — *Rotation resulted into a research paper*

Professional Service

To discipline

- 2010-Present Associate Faculty Member, Faculty 1000 Biology
- 2003-Present Reviewer for over 10 scientific journals, including Plos Computation Biology, Proteins: Structure, Function, and Bioinformatics, FEBS Letter, Biochemistry, and Biophysical Journal

Professional Affiliation

- 2006-Present International Society for Computational Biology
- 2005-2006 Protein society
- 2000-2003 American Physical Society

Grants

Ongoing

2007-2012 National Institutes of Health

Protein misfolding and aggregation (PI: Nikolay V. Dokholyan)

Role: Co-investigator

2011-2015 Defense Threat Reduction Agency

Novel bioscavengers against OP nerve agents (PI: Nikolay V. Dokholyan)

Role: Co-Principle investigator

Completed

2009-2011 University Research Council Small Grant Program, UNC CH

Computational design of *de novo* peptide binding to specific target proteins (PI: Feng Ding)

Role: Principle investigator

2009-2011 National Institutes of Health

Retroviral Genomic RNA Dimer Structure and Function-ARRA (PI: Kevin M. Weeks)

Role: Co-Investigator