Jeffrey K. Noel

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www: SMOG webpage (http://smog-server.org/noel)

Education

Ph.D. in Physics	University of California, San Diego	June 15, 2012
Master of Science	University of California, San Diego	June 15, 2007
Bachelor of Science	University of Wisconsin, Madison	June 6, 2005
	Major: Applied Math, Engineering, and Physics (Computer Engineering focus)	

Research Experience

Humboldt Fellow — Max Delbrück Center and Fritz Haber Institute, Berlin — 2015–Present

Postdoctoral Fellow — Center For Theoretical Biological Physics, Rice University — 2013–2015

Worked on structure-function relationships in large scale biomolecular conformational rearrangements, including the conformational transition of influenza surface protein hemagglutinin during membrane fusion, and the molecular details of kinetic proofreading in the ribosome during tRNA accommodation.

Graduate Research (Dr. José Onuchic) — Physics Department, University of California, San Diego — 2006–2012

Thesis title: Development and Application of All-Atom Structure-based Models for Studying the Role of Geometry in Biomolecular Folding and Function. [PDF]

Developed an all-atom structure-based model and applied it to protein folding and function. Showed that the folding of knotted proteins likely includes "slipknotted" intermediates with the first thermodynamic sampling of a knotted protein.

Co-creator of http://smog-server.org, a webtool and tutorial aiding the creation of structure-based models.

Awards and Honors

Guest Researcher of the Max Planck Society	2015-2017
Alexander von Humboldt Postdoctoral Fellowship	2015-2017
Robert A. Welch Foundation Postdoctoral Fellow	2014-2015
NIH Molecular Biophysics Training Grant	2007–2009
San Diego Fellowship	2005–2007

Computing Awards

XSEDE Grant MCB140274 for 4.6MSUs (Co-PI)	2014
National Research Council (NRC) Anton Grants PSCA00062P, PSCA14037P, and PSCA15061P (Co-PI)	2011/2014/2015

Peer-Reviewed Publications (including peer-reviewed review articles)

26. Fisher KM, Haglund E, **Noel JK**, Hailey KL, Onuchic JN, Jennings PA (2015) Geometrical frustration in Interleukin-33 decouples the dynamics of the functional element from the folding transition state ensemble. PLOS One (in press) [link]

25. **Noel JK**, Morcos F, Onuchic JN (2015) Sequence co-evolutionary information is a natural partner to minimally-frustrated models of biomolecular dynamics. F1000 (in press) [link]

24. Lammert H, **Noel JK**, Haglund E, Schug A, Onuchic JN (2015) Constructing a folding model for protein S6 guided by native fluctuations deduced from NMR structures (under review) [link]

23. Ramirez-Sarmiento CA, **Noel JK**, Valenzuela SL, Artsimovitch I (2015) Interdomain contacts control native state switching of RfaH on a dual-funneled landscape. PLOS Comp. Biol. 11, e1004379. [link]

22. Cheng RR, Raghunathan M, **Noel JK**, Onuchic JN (2015) Constructing sequence-dependent protein models using coevolutionary information. Protein Science [link]

21. Hayes RL, **Noel JK**, Mandic A, Whitford PC, Udayan M, Sanbonmatsu KY, Onuchic JN (2015) Generalized Manning Condensation Model Captures the RNA Ion Atmosphere. Phys. Rev. Lett. 114, 258105. [link]

20. Sun L, **Noel JK**, Sulkowska JI, Levine H, Onuchic JN (2014) Connecting thermal and mechanical protein (un)folding landscapes. Biophys. J. 107, 2941-52. [link]

19. **Noel JK**, Chahine J, Leite VBP, Whitford PC (2014) Capturing Transition Paths and Transition States for Conformational Rearrangements in the Ribosome. Biophys. J. 107, 2872-81. [link]

18. Lin X, Eddy NR, **Noel JK**, Whitford PC, Wang Q, Ma J, Onuchic JN (2014) Order and disorder control the functional rearrangement of influenza hemagglutinin. PNAS 111(33):12049-54. [link]

17. Haglund E, Sulkowska JI, **Noel JK**, Lammert H, Onuchic JN, Jennings PA (2014) Pierced Lasso Bundles are a New Class of Knot Motifs. PLOS Comp. Biol. 10(6): e1003613. [link]

16. **Noel JK**, Whitford PC (2014) How Simulations Reveal Dynamics, Disorder, and the Energy Landscapes of Biomolecular Function. Isr. J. Chem., 54(8-9), 1093–107. [link]

15. Hayes RL, **Noel JK**, Whitford PC, Udayan M, Sanbonmatsu KY, Onuchic JN (2014) Reduced Model Captures Mg2+-RNA Interaction Free Energy of Riboswitches. Biophys. J. 106(7) 1508-19. [link]

14. *Ozenne V, ***Noel JK**, Heidarsson PO, Brander S, Poulsen FM, Jensen MR, Kragelund BB, Blackledge M, Danielsson J (2014) Exploring the minimally frustrated energy landscape of unfolded ACBP. J. Mol. Biol. 426(3) 722-34. [link]

13. **Noel JK**, Onuchic JN, Sulkowska JI (2013) Knotting a protein in explicit solvent. J. Phys. Chem. Lett. 4(21) 3570-3. [link]

12. Lammert H, **Noel JK**, Onuchic JN (2012) The Dominant Folding Route Minimizes Backbone Distortion in SH3. PLOS Comput Biol 8(11): e1002776. [link]

11. *Sulkowska JI, ***Noel JK**, Onuchic JN (2012) Energy landscape for knotted protein folding. (2012) PNAS 109 17783−88. [link]

10. Hayes RL, **Noel JK**, Mohanty U, Whitford PC, Hennelly SP, Onuchic JN, Sanbonmatsu KY (2012) Magnesium Fluctuations Modulate RNA Dynamics in the SAM-I Riboswitch. J. Amer. Chem. Soc. 134(29):12043-53. [link]

9. **Noel JK**, Whitford PC & Onuchic JN (2012) The Shadow Map: A General Contact Definition for Capturing the Dynamics of Biomolecular Folding and Function. Journal of Physical Chemistry B, 116, 8692−8702. [link]

8. **Noel JK**, Schug A, Verma A, Wenzel W, Garcia AE & Onuchic JN (2012) Mirror images as naturally competing conformations in protein folding. Journal of Physical Chemistry B, 116, 6880-8. [link]

7. *Suzuki Y, ***Noel JK** & Onuchic JN, (2011) A semi-analytical description of protein folding that incorporates detailed geometrical information. Journal of Chemical Physics 135 245101. [link]

6. **Noel JK**, Sułkowska JI & Onuchic JN (2010) Slipknotting upon Native-like Loop Formation in a Trefoil Knot Protein. PNAS 107 (35) 15403-15408. [link]

5. **Noel JK**, Whitford PC, Sanbonmatsu KY & Onuchic JN (2010) SMOG@ctbp: simplified deployment of

structure-based models in GROMACS. Nucleic Acids Research 38 W657–61. [link]

4. Whitford PC, **Noel JK**, Gosavi S, Schug A & Onuchic JN (2009) An All-atom Structure-Based Potential for Proteins: Bridging Minimal Models with Empirical Forcefields. Proteins: Structure, Function, Bioinformatics. 75 (2) 430-441. [link]

3. Suzuki Y, **Noel JK** & Onuchic JN (2008) An analytical study of the interplay between geometrical and energetic effects in protein folding. Journal of Chemical Physics. 128 025101-(1-6). [link]

2. Vano JA, Wildenberg JC, Anderson MB, **Noel JK** & Sprott JC (2006) Chaos in low-dimensional Lotka-Volterra models of competition. Nonlinearity. 19 (10) 2391-2404. [link]

1. Sprott JC, Vano JA, Wildenberg JC, Anderson MB & **Noel JK** (2005) Coexistence and chaos in complex ecologies. Physics Letters A. 335 (2-3) 207-212. [link]

* shared first author

Reviews and Chapters

4. **Noel JK**, Morcos F, Onuchic JN (2015) Sequence co-evolutionary information is a natural partner to minimally-frustrated models of biomolecular dynamics. F1000 (under review) [link]

3. **Noel JK**, Whitford PC (2014) How Simulations Reveal Dynamics, Disorder, and the Energy Landscapes of Biomolecular Function. Isr. J. Chem., 54(8-9), 1093–107. [link]

2. Sulkowska JI, **Noel JK**, Ramirez-Sarmiento CA, Rawdon EJ, Millett KC, Onuchic JN (2013) Knotting pathways in proteins. Biochemical Society Transactions 41, 523–527. [link]

1. **Noel JK** & Onuchic JN, The many faces of structure-based potentials: From protein folding landscapes to structural characterization of complex biomolecules. Chapter 2 in Computational Modeling of Biological Systems; Dokholyan, N. Ed., Springer: New York, 2012. [link]