

JEFFREY K. NOEL, PH.D.

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EDUCATION

Ph.D. in Physics University of California, San Diego June 15, 2012
Thesis title: Development and Application of All-Atom Structure-based Models for
Studying the Role of Geometry in Biomolecular Folding and Function
Bachelor of Science University of Wisconsin, Madison June 6, 2005
Major: Applied Math, Engineering, and Physics (Computer Engineering focus)

RESEARCH EXPERIENCE

Postdoc, Max-Delbrück Center, Berlin (PI: Oliver Daumke and Alexander Mikhailov) 2016-Present

- Using various techniques (soft matter physics, all-atom simulations, coarse-grained simulations, biochemical experiments) to understand the molecular mechanism of the dynamin molecular motor, a polymeric GTPase machine that catalyzes membrane scission during endocytosis.

Postdoctoral Fellow, Center for Theoretical Biological Physics, Rice University (PI: José Onuchic) 2013-2015

- Applied all-atom structure-based models and explicit solvent simulations to study large-scale molecular rearrangements in the ribosome and influenza hemagglutinin

AWARDS AND HONORS

Alexander von Humboldt Postdoctoral Fellowship 2016-2018
Guest Researcher of the Max Planck Society 2015-2018
Robert A. Welch Foundation Postdoctoral Fellow 2014-2015
NIH Molecular Biophysics Training Grant 2007-2009
San Diego Fellowship 2005-2007
AMEP Leadership Award 2005
NSF REU Grant 2003 & 2004

Computing Awards

XSEDE Grant MCB140274 for 4.6MSUs (Co-PI) 2014
**National Research Council (NRC) Anton Grants PSCA00062P, PSCA14037P,
PSCA15061P, and PSCA16067P** (Co-PI) 2011-2017

PEER-REVIEWED PUBLICATIONS (INCLUDING PEER-REVIEWED REVIEW ARTICLES)

* shared authorship # corresponding author

37. Danielsson J, **Noel, JK**, Duggan B, Oliveberg M, Onuchic JN, Jennings PA, Haglund E (2020) The pierced lasso topology leptin has a bolt on dynamic domain composed by the disordered loops I and III. *J. Mol. Bio.*, 432, 3050-63. [[link](#)]
36. #**Noel JK**, Noé F, Daumke O, and Mikhailov AS (2019) Polymer-like model to study the dynamics of dynamin filaments on deformable membrane tubes. *Biophys. J.* 117, 1870-91. [[link](#)]
35. Faelber K, Dietrich L, ***Noel JK**, *F Wollweber, *A-K Pfitzner, et al., M van der Laan, W Kuhlbrandt, and O Daumke (2019) Structure and assembly of the mitochondrial membrane remodelling GTPase Mgm1. *Nature* 571, 429-33. [[link](#)]
34. Levi M, #**Noel JK**, #Whitford PC (2019) Studying ribosome dynamics with simplified models. *Methods*, 162,

128-40. [\[link\]](#)

33. Liu JW, **Noel JK**, Low, HH (2018) Structural basis for membrane tethering by a bacterial dynamin-like pair. *Nature Comms.*, 9, 3345. [\[link\]](#)

32. Lin X, **Noel JK**, Wang Q, Ma J, Onuchic JN (2018) Atomistic Simulations of the Loop to Coiled-Coil Functional Transition of the B-loop Domain of Influenza Hemagglutinin. *Proc. Natl. Acad. Sci. USA* 115, E7905–E7913. [\[link\]](#)

31. Sun L, **Noel JK**, Levine H, Onuchic JN (2017) Molecular simulations suggest a force-dependent mechanism of vinculin activation. *Biophys. J.* 113(8), 1697–710. [\[link\]](#)

30. Yang H, **Noel JK**, Whitford PC (2017) Anisotropic Fluctuations in the Ribosome Determine tRNA Kinetics. *J. Phys. Chem. B* 121, 10593-601 [\[link\]](#)

29. **Noel JK**, Whitford PC (2016) How EF-Tu can enable efficient proofreading of aa-tRNA by the ribosome. *Nature Comms.* 7, 13314. [\[link\]](#)

28. *Lin X, ***Noel JK**, Wang Q, Ma J, Onuchic JN (2016) Lowered pH Leads to Fusion Peptide Release and a Highly-dynamic Intermediate in Influenza Hemagglutinin. *J. Phys. Chem. B* 120, 9654–60. [\[link\]](#)

27. **Noel JK**, Levi M, Raghunathan M, Lammert H, Hayes RL, Onuchic JN, Whitford PC (2016) SMOG 2: A Versatile Software Package for Generating Structure-Based Models. *PLOS Comput. Biol.* 12, e1004794. [\[link\]](#)

26. **Noel JK**, Morcos F, Onuchic JN (2016) Sequence co-evolutionary information is a natural partner to minimally-frustrated models of biomolecular dynamics. *F1000Res* 5, 1-7. [\[link\]](#)

25. Cheng RR, Raghunathan M, **Noel JK**, Onuchic JN (2016) Constructing sequence-dependent protein models using coevolutionary information. *Protein Sci.* 25, 111–22. [\[link\]](#)

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. *J. Chem. Phys.* 143, 243141. [\[link\]](#)

23. 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* 10, e0144067. [\[link\]](#)

22. 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. [\[link\]](#)

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. *Proc. Natl. Acad. Sci. USA*, 111, 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: e1003613. [\[link\]](#)

16. **Noel JK**, Whitford PC (2014) How Simulations Reveal Dynamics, Disorder, and the Energy Landscapes of Biomolecular Function. *Isr. J. Chem.*, 54, 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, 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, 722-34. [\[link\]](#)
13. **Noel JK**, Onuchic JN, Sulkowska JI (2013) Knotting a protein in explicit solvent. *J. Phys. Chem. Lett.* 4, 3570-3. [\[link\]](#)
12. Lammert H, **Noel JK**, Onuchic JN (2012) The Dominant Folding Route Minimizes Backbone Distortion in SH3. *PLOS Comput. Biol.* 8, e1002776. [\[link\]](#)
11. *Sulkowska JI, ***Noel JK**, Onuchic JN (2012) Energy landscape for knotted protein folding. (2012) *Proc. Natl. Acad. Sci. USA*, 109, 17783–88. [\[link\]](#)
10. Hayes RL, **Noel JK**, Mohanty U, Whitford PC, Hennelly SP, Onuchic JN, Sanbonmatsu K (2012) Magnesium Fluctuations Modulate RNA Dynamics in the SAM-I Riboswitch. *J. Amer. Chem. Soc.*, 134, 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. *J. Phys. Chem. 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. *J. Phys. Chem. 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. *J. Chem. Phys.*, 135, 245101. [\[link\]](#)
6. **Noel JK**, Sulkowska JI & Onuchic JN (2010) Slipknotting upon Native-like Loop Formation in a Trefoil Knot Protein. *Proc. Natl. Acad. Sci. USA*, 107, 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 Res.* 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.* 75 430-441. [\[link\]](#)
3. Suzuki Y, **Noel JK** & Onuchic JN (2008) An analytical study of the interplay between geometrical and energetic effects in protein folding. *J. Chem. Phys.*, 128 025101. [\[link\]](#)
2. Vano JA, Wildenberg JC, Anderson MB, **Noel JK** & Sprott JC (2006) Chaos in low-dimensional Lotka-Volterra models of competition. *Nonlinearity.* 19, 2391-2404. [\[link\]](#)
1. Sprott JC, Vano JA, Wildenberg JC, Anderson MB & **Noel JK** (2005) Coexistence and chaos in complex ecologies. *Phys. Let. A*, 335 (2-3) 207-212. [\[link\]](#)

REVIEWS AND CHAPTERS

5. Levi M, Bandarkar P, Yang H, Wang A, Mohanty U, **Noel JK**, Whitford PC (2018) Using SMOG 2 to simulate complex biomolecular assemblies. Chapter in: *Methods in Molecular Biology*, Springer Nature (in press) [\[link\]](#)
4. **Noel JK**, Morcos F, Onuchic JN (2016) Sequence co-evolutionary information is a natural partner to minimally-frustrated models of biomolecular dynamics. *F1000Res* 5, 1-7. [\[link\]](#)
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. [\[link\]](#)