

# JEFFREY K. NOEL, PH.D.

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## EDUCATION

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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

## RESEARCH EXPERIENCE

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Postdoc, Max-Delbrück Center, Berlin (PI: Oliver Daumke and Alexander Mikhailov)	2016-
Postdoctoral Fellow, Center for Theoretical Biological Physics, Rice University (PI: José Onuchic)	2013-2015

## AWARDS AND HONORS

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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

### 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

## WORKSHOPS CO-ORGANIZED

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RNA Dynamics: Going from In Vitro to In Silico. RNA Institute Workshop, Albany, NY	Mar 2015
Structure-based Models with SMOG@ctbp. International Conference on Biological Physics, San Diego, CA	Jun 2011
Protein Dynamics: Going from In Vitro to In Silico: A Center for Theoretical Biological Physics Workshop. University of California, San Diego, CA	May 2007

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

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33. Liu JW, **Noel JK**, Low, HH (2018) Structural basis for membrane tethering by a bacterial dynamin-like pair. *Nature Communications*, 9(1), 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. *PNAS* 115(34), 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(3): 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 Science* 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(12): 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. *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 Mg<sup>2+</sup>-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

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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. Sułkowska 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. [\[link\]](#)

## INVITED TALKS

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“Toward understanding the dynamin molecular motor: a molecular python” Centre of New Technologies Seminar, Warsaw, Poland	Mar 2018
“Using molecular simulation to understand the interplay between molecular machine geometry and the kinetics of conformational changes” Neuroscience Dept, Okayama, Japan	Mar 2018
“Using molecular simulation to understand the interplay between molecular machine geometry and the kinetics of conformational changes” NanoLSI Seminar, Kanazawa, Japan	Mar 2018
“The operation of the dynamin molecular motor” 9th International Conference Engineering of Chemical Complexity, Barcelona, Spain	Jun 2017
“How EF-Tu Can Contribute to Efficient Proofreading of aa-tRNA by the Ribosome” Huenfeld Theory 2017, Huenfeld, Germany	Mar 2017
“Connecting tRNA accommodation, EF-Tu dissociation, and kinetic proofreading in the ribosome.” 6th Visegrad Symposium on Structural Systems Biology, Warsaw, Poland	Jun 2016
“Kinetic proofreading in the ribosome: Probing the free-energy landscape of fidelity” Kyoto University, Kyoto, Japan	Mar 2016
“Kinetic proofreading in the ribosome: Probing the free-energy landscape of fidelity” Hiroshima University, Hiroshima, Japan	Mar 2016
“Enriching structure-based models with coevolutionary information” New Frontiers in Nonlinear Sciences Workshop, Niseko, Japan	Mar 2016
“Energy Landscapes of Biomolecular Machines: Capturing Transition Paths for Conformational Rearrangements in the Ribosome” BCSCCS Seminar, Fritz-Haber Institute, Berlin	Nov 2015
“Enriching structure-based models with coevolutionary information” Protein Folding Consortium Meeting, Berkeley, CA	May 2015
“Free energy landscape of tRNA accommodation in the ribosome” Max Delbrück Center, Berlin, Germany	Jan 2015
“Understanding knotted protein folding by combining coarse-grained and explicit solvent simulations” Biophysical Society Meeting: The Significance of Knotted Structures for the Function of Proteins and Nucleic Acids, Warsaw, Poland	Sept 2014
“The Massive Functional Rearrangement of Influenza Hemagglutinin” ACS Fall Meeting, San Francisco	Aug 2014
“Characterizing the Energy Landscape of tRNA Accommodation in the Ribosome” 1st Symposium on Current Topics in Molecular Biophysics, University of Sao Paulo, Brazil	May 2014
“Structure-based models: Versatile models for studying protein folding and function through energy landscape theory” University of Chile, Santiago, Chile	May 2014
“How protein folding is teaching us about molecular machines” Frontiers in Science Seminar Series, University of Houston, Houston, TX	Mar 2014
“Folding of topologically complex proteins: slipknots and lassos” CIBR, Baylor College of Medicine, Houston, TX	Feb 2014
“Understanding knotted protein folding” Physics Seminar, Northeastern University, Boston, MA	Jul 2013
“Detailed simulations of protein slipknotting events during folding” Protein Folding Consortium Meeting, Berkeley, CA	May 2013
“Studying biomolecular dynamics using structure-based potentials with SMOG,” SCC seminar, Karlsruhe Institute of Technology, Karlsruhe, Germany	Sep 2012
“Studying biomolecular dynamics using structure-based potentials with SMOG,” TCB Seminar, Beckman Institute, Urbana, IL	Aug 2012

- “Structure-based Models with SMOG@ctbp: From Protein Folding Landscapes to Structural Characterization of Complex Biomolecules,” International Conference on Biological Physics, La Jolla, CA Jun 2011
- “Folding a Trefoil Knot Protein,” Topological Problems in Molecular Biology, American Mathematical Society Meeting, Iowa City, Iowa Mar 2011
- “Entropy, Symbolic Dynamics, and Dynamical Systems,” Chaos and Complex Systems Seminar, University of Wisconsin, Madison Apr 2005