Eric R. Beyerle

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Research Interests

Statistical mechanics of biological systems; data-driven reaction coordinate discovery; close-to-equilibrium dynamics of biological systems; physics- and chemistry-intelligent machine learning (both deep and non-deep)

Education

Ph.D, University of Oregon 2015-2021
Department of Chemistry Eugene, Oregon
Advisor: Marina Guenza
Dissertation: Extensions of the Langevin Equation for Protein Dynamics for Modelling Equilibrium Fluctuations of Proteins

B.S., Centre College 2011-2015
Major: Chemical Physics
Minor: Chemistry Danville, Kentucky

Work Experience

Postdoctoral Associate with Prof. Kresten Lindorff-Larsen, University of Copenhagen Department of Biology; University of Copenhagen, Copenhagen, Denmark; 1 September 2024 to present

Postdoctoral Associate with Prof. Pratyush Tiwary, Institute for Physical Science and Technology; University of Maryland, College Park 1 September 2021 to 31 August 2024

Undergraduate researcher for Prof. Yong Li, Department of Biochemistry and Molecular Biology, University of Louisville 15 June 2013 to 1 September 2013

Eric Beyerle

Undergraduate researcher for Prof. Steve Asmus, Biochemistry and Molecular Biology and Biology Programs, Centre College 15 June 2012 to 1 September 2012

Awards

1. ACS COMP Wiley Computers in Chemistry Outstanding Postdoc Award, Spring 2024

2. John Keana Fellow, University of Oregon, 2019

3. Valedictorian Prize, Centre College, 2015

4. Max P Cavnes Award, Centre College, 2012

5. Walkup-Barton Grant, Centre College, 2012

6. Faculty Scholarship, Centre College, 2011-2015

Publications

1. Akashnathan Aranganathan and E. R. Beyerle, "Kinetics and dynamics directly from AlphaFold2," manuscript in preparation

2. E. R. Beyerle and P. Tiwary, "Inferring the Isotropic-nematic Phase Transition with Generative Machine Learning," arXiv:2410.21034v1; accepted for publication at *Phys. Rev. Lett.*

3. D. Wang, Y. Qiu, E. R. Beyerle, X. Huang, and P. Tiwary, "An information bottleneck approach to Markov state model construction," *J. Chem. Theory Comput.* **20**, 5352-5367, 2024

4. E. R. Beyerle and P. Tiwary, "Thermodynamically inspired machine-learned reaction coordinates for hydrophobic ligand dissociation," *J. Phys. Chem B*, **128**, 3, 755-767, 2024

5. K. Choudhary *et al.*, "Large Scale Benchmark of Materials Design Methods," *npj Computational Materials*, **10**, 93, 2024

6. E. R. Beyerle, Z. Zou, an P. Tiwary, "Recent advances in describing and driving crystal nucleation using machine learning and artificial intelligence," *Current Opinion in Solid State & Materials Science*, **27**, 2023

7. Z. Zou*, E. R. Beyerle*, S. Tsai, and P. Tiwary, Driving and characterizing nucleation of urea and glycine polymorphs in water, *PNAS,* 7, 120, 2023. *joint first author with Z. Zou

8. E. R. Beyerle, S. Mehdi, and P. Tiwary. Quantifying Energetic and Entropic Pathways in Molecular Systems. *J. Phys. Chem. B.*, **126**, 21, 3950-3960, 2022.

9. E. R. Beyerle and M. G. Guenza. Identifying the leading dynamics of ubiquitin: a comparison between the tICA and the LE4PD slow fluctuations in amino acids' position. *J. Chem. Phys.*, **155**, 244108, 2021.

10. E. R. Beyerle. Extensions of the Langevin Equation for Protein Dynamics for Modelling Equilibrium Fluctuations of Proteins. Ph.D dissertation. University of Oregon, 2021.

11. E. R. Beyerle and M. G. Guenza. Comparison between slow, anisotropic LE4PD fluctuations and the Principal Component Analysis modes of Ubiquitin. *J. Chem. Phys.*, 154, 12411, 2021. Paper published as part of the Special Collection in Honor of Women in Chemical Physics and Physical Chemistry.

12. E. R. Beyerle, M. Dinpajooh, H. Ji, P. von Hippel, A. H. Marcus, and M. G. Guenza. Dinucleotides as simple models of the base stacking-unstacking component of DNA 'breathing' mechanisms. *Nucleic Acids Research,* 49, 1872 - 1885, 2021

13. E. R. Beyerle and M. G. Guenza. Kinetic Analysis of Ubiquitin Local Fluctuations with Markov State Modeling of the LE4PD Normal Modes. *J. Chem. Phys.*, 151(16):164119, 2019. Paper published as part of the Special Collection on Markov Models and Molecular Kinetics.

14. Copperman, J.; Dinpajooh, M.; Beyerle, E.; Guenza, M. Universality and specificity in protein fluctuation dynamics. *Phys. Rev. Lett.*, 119, 158101 , 2017.

15. Asmus, S.; Raghanti, M.; Beyerle, E.; Fleming-Beattie, J.; Hawkins, S.; McKernan, C.; and Rauh, N. Tyrosine hydroxylase-producing neurons in the human cerebral cortex do not colocalize with calcium-binding proteins or the serotonin 3A receptor. *J. Chem. Neuroanat.* **78**, 1-9, 2016.

Invited Talks

1. LCB Seminar, NIH, 1 February 2024

2. Statistical Thermodynamics and Molecular Simulations (STMS) virtual seminar series, 27 October 2023

3. Informal Statistical Physics Seminar, University of Maryland, 26 September 2023

Presentations

1. *Learning Thermodynamics and Reaction Coordinates for Colloidal Phase Transitions*, IMSI workshop on collective variables and coarse graining, April 23rd, 2024; Poster

2. *Thermodynamically optimized reaction coordinates for hydrophobic ligand* unbinding, ACS Spring Meeting in New Orleans, March 19th, 2024; Poster

3. *Thermodynamically optimized reaction coordinates for hydrophobic ligand* unbinding, Gordon research conference on protein folding, January 8th, 2024; Poster

4. *Machine-learned reaction coordinates for hydrophobic ligand binding*, iPOLS meeting, August 1st, 2023, Talk

5. *Machine-learned reaction coordinates for energy-entropy disentanglement*, Brin workshop on rare events, February 27th, 2023, Talk

6. *A Comparison of the Slow Dynamics in the Protein Ubiquitin Predicted by the LE4PD, PCA, and tICA from a Long Equilibrium Molecular Dynamics Simulation.* APS March Meeting, March 16th, 2021 (Virtual), Talk.

7. *Kinetics Analysis of Protein Fluctuations with Markov State Modeling of LE4PD Normal Modes.* Northwest Theoretical and Computational Chemistry Conference, June 15th, 2019, Talk.

8. *An Anisotropic Langevin Equation for Protein Dynamics.* Annual Meeting of the APS, March 4th , 2019, Talk.

9. *The Influence of Free-energy Surfaces on Protein Dynamics.* Engineering Biomolecules Mini-Symposium, June 22nd , 2018, Poster.

10. *The Influence of Free-energy Surfaces on Protein Dynamics.* Annual Meeting of the APS Northwest Section, June 2nd , 2018, Talk.

11. *A Comparison of Collective Coordinates for Analyzing Protein Dynamics.* Biophysical Society Annual Meeting, February 19th , 2018, Poster.

12. *A Study of Internal Friction in Ubiquitin Using a Diffusive, Langevin Formalism.* Annual Meeting of the APS Northwest Section, June 2nd , 2017, Talk.

13. *Exploring Protein Dynamics Using a Diffusive, Langevin Formalism.* OMQ Open House, March 2017, Poster.

14. *A Chemical Examination of an Oil Painting in the Evans-Lively Room.* RICE Symposium, April 2015, Poster.

15. *The Calcium-binding Proteins Calbindin, Calretinin, and Parvalbumin Do not Colocalize with Tyrosine Hydroxylase in Brodmann's Areas 10 and 24 of the Human Cerebral Cortex.* RICE Symposium, April 2013, Poster.

16. *An Examination of the Linguistics of New Mexican Spanish.* RICE Symposium, April 2013, Talk.

Teaching Experience

1. Both teacher and teaching assistant for a Python summer bootcamp hosted at UMD by Prof. Pratyush Tiwary in the summers of 2024 and 2025

2. Teaching assistant for CH 411 (physical chemistry; instructor: Prof. Marina Guenza); University of Oregon, Fall 2020 [online due to COVID-19 pandemic]

3. Teaching assistant for CH 447 (computational chemistry; instructor: Prof. Marina Guenza); University of Oregon, Fall 2016 and Fall 2017

4. Section instructor for CH 227, 228, and CH 229 (general chemistry laboratory); total of seven (7) quarters of teaching experience; University of Oregon, 2015-2018

5. Section instructor for CH 399 (honors general chemistry laboratory, research immersion); University of Oregon, 2018-2019

6. Teaching assistant for CHE 241 and CHE 242 (organic chemistry I & II; instructor: Prof. Joe Workman); Centre College, Fall 2014 and Spring 2015

University Service

1. Postdoctoral mentor in the graduate student – postdoc mentoring program for a semester at UMD, Spring 2024

2. Poster and Presentation Judge for the GRAD symposium at the University of Maryland, College Park, April 11th, 2024

3. Referee for *Journal of Chemical Information and Modelling*, *Journal of Chemical Theory and Computation*, *The Journal of Physical Chemistry B, Soft Matter*, *Molecular Simulation*, *Computational Biology and Chemistry*, and *Proteins: Structure, Function, and Bioinformatics*

4. Jobs panel, 2023 iPOLS meeting, 1 August 2023

5. Undergraduate mentor to Sonny Kusaka and Ruben Sanchez at the University of Oregon, 2019-2021

6. Physics tutor, Centre College Department of Physics, 2014-2015

Extracurricular

1. Coordinator (Treasurer in 2019-2020; President in 2020-2021) for the University of Oregon running club; also webmaster from 2019-2023

Professional References

Pratyush Tiwary
Millard and Lee Alexander Professor in Chemical Physics
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Marina Guenza
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