DEDI WANG

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EDUCATION

University of Maryland, College Park, MD, USA *Aug 2019-May 2024 (expected)*
PhD candidate, Biophysics

Peking University, Beijing, China *Sep 2015-Jun 2019*
B.S., Physics GPA: 3.71/4.0

RESEARCH INTERESTS

Complex Systems, Drug Discovery, Molecular Dynamics Simulation,
Statistical Mechanics, Representation Learning & Artificial Intelligence (AI)

RESEARCH EXPERIENCE

Department of Chemistry & Biochemistry, University of Maryland *Sep 2019 – Present*
Research Assitant *Advisor:* ***Pratyush Tiwary***

- **Physics-informed representation learning methods for dynamical systems**
  Capitalized on physics-inspired insights to learn useful but also meaningful low dimensional representations of the deluge of data generated from experiments and simulations, providing mechanistic insights across various domains of chemical and biological physics.

- **AI augmented molecular dynamics (MD) that reach experimental timescales**
  Developed AI augmented molecular dynamics (MD) methods that allow for studying complex molecular systems across an extensive range of timescales, from femtoseconds to seconds, while preserving all-atom resolution.

Cancer Data Science Lab, NCI, NIH *Nov 2019 – Jan 2020*
Research Rotation *Advisor:* ***Sridhar Hannenhalli***

- **Identifying genes with distinct functions across different tissues**
  Applied the network diffusion to tissue-specific netwroks to get ”complete” tissue-specific GO annotations, developed a metrics to find out tissue-dependent genes which shed light on the underlying mechanism of some complex diseases.

Center of Quantitative Biology, Peking University *Jan 2017 – Jun 2019*
Undergraduate Research Assistant *Advisor:* ***Fangting Li***

- **The Global Dynamic Stability in Budding Yeast Cell Cycle**
  Built an auto-evolving simplified ODE model, developed new tools to analyze complex dynamic system, and proposed a promising mechanism that provides the cell-cycle process with a sufficient duration for each event and an attractive manifold for the state checking.

PUBLICATIONS

Wang, D., Wang, Y., Evans, L. and Tiwary, P., 2022. From latent dynamics to meaningful representations. arXiv preprint arXiv:2209.00905.

Vani, B.P., Aranganathan, A., **Wang, D.**. and Tiwary, P., 2022. AlphaFold2-RAVE: From Sequence to Boltzmann Ranking. Journal of Chemical Theory and Computation.

Mehdi, S., **Wang, D.**, Pant, S. and Tiwary, P., 2022. Accelerating all-atom simulations and gaining mechanistic understanding of biophysical systems through state predictive information bottleneck. Journal of Chemical Theory and Computation, 18(5), pp.3231-3238.

Wang, D., Zhao, R., Weeks, J.D. and Tiwary, P., 2022. Influence of Long-Range Forces on the Transition States and Dynamics of NaCl Ion-Pair Dissociation in Water. The Journal of Physical Chemistry B, 126(2), pp.545-551.

Wang, D. and Tiwary, P., 2021. State predictive information bottleneck. The Journal of Chemical Physics, 154(13), p.134111.

Wang, D., Zhao, Y., Zhang, Z., Lu, Y., Yang, X., Ouyang, Q., Tang, C. and Li, F., 2020. Critical slowing down and attractive manifold: A mechanism for dynamic robustness in the yeast cell-cycle process. Physical Review E, 101(4), p.042405.

SELECTED HONORS AND AWARDS

Ann Wylie Dissertation Fellowship, University of Maryland, College Park	*Mar 2023*
Outstanding Research Assistant Award, University of Maryland, College Park	*Jan 2022*
Award for Scientific Research, Peking University	*Dec 2018*
May 4th Scholarship, Peking University	*Dec 2018*
Award for Academic Excellents, Peking University	*Dec 2017*
Award for Academic Deligence, Peking University	*Dec 2016*
May 4th Scholarship, Peking University	*Dec 2016*

ACADEMIC ACTIVITIES

MolSSI Workshop *May 2023*
Machine Learning and Chemistry: Are We There Yet?

- Poster: ”Unlocking the Power of Molecular Dynamics with Physics-Informed Representation Learning”

Brin MRC Workshop *Feb 2023*
Rare Events: Analysis, Numerics, and Applications

- Talk: ”Introducing Physics into representation learning”

Protein Folding Dynamics Gordon Research Conference *Oct 2022*

- Poster: ”Capturing Protein Conformational Dynamics through Information Bottleneck and Molecular Dynamics”

Protein Folding Dynamics Gordon Research Seminar *Oct 2022*

- Talk and poster: ”Capturing Protein Conformational Dynamics through Information Bottleneck and Molecular Dynamics”

American Physical Society March Meeting *Mar 2021*

- Talk: ”State Predictive Information Bottleneck”

MENTORING ACTIVITIES

Graduate students:

1. Jessica Bodosa
2. Shams Mehdi
3. Ryan Nival
4. Vanessa Meraz
5. Suemin Lee

Undergraduate student:

1. Fiona Mon