Rui Guo

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SKILLS

- Intermediate level of coding in C++ (familiar with STL data structures and object orienting programing) and python (data analysis and visualization with numpy, pandas and matplotlib). [6+ years]
- Familiar with programming tools including command line, shell scripting, vim and git. Experienced with basic maintenance of high-performance Linux clusters. [6+ years]
- Extensive experience with computational protein design (protein sequence prediction/reverse protein folding problem), solving the design problem by applying a statistical entropy model written in C++. [6+ years]
- High capability of performing molecular dynamics simulations of protein systems with NAMD. [6+ years]
- Expert at protein visualizations with VMD & Pymol, familiar with techniques such as drawing methods, lighting and materials, renderings of electrostatic surface and heat maps, and protein animations. [6+ years]
- Knowledgeable of applying physical models to interpret protein experimental data (e.g. fitting thermal melting temperature and enthalpy; calculating protein PI and charge-PH relations). [5+years]
- Bioinformatics/Genomics – Coursera courses: Introduction to Genomics Technologies; Python for Genomic Data Science; Algorithms for DNA sequences; Command Line Tools for Genomics.

EDUCATION

University of Pennsylvania **Expected May 2023**
Ph.D., Physical Chemistry - GPA: **3.90/4.0** **Advisor: Dr. Jeffery Saven**
Thesis: Computational engineering of protein features: charge variation, host-guest assembly, and structural motif.

University of Science and Technology of China (Hefei) **Jun 2016**
B.S., Chemistry – GPA: **3.63/4.3** **Advisor: Dr. Tongwen Xu**

- Outstanding Student Scholarship for 4 years **(**2015 – grade 1 scholarship, top 3%; 2014 & 2013 – grade 2 scholarship top 10%; 2012 – grade 3 scholarship, top 25%)

RESEARCH EXPERIENCE

Graduate Research Associate - University of Pennsylvania **Jan 2017 - 2023**

Focus: *Applying a statistical model to solve the protein design problem, i.e., calculating amino acid sequences that when synthesized, fold into target 3D protein structures, to create proteins that possess desired functionalities, such as high thermal stability, enzyme activity or host-guest assemblies.*

- **Computational Protein Design** (2 projects • 18 designed proteins • 16 confirmed to fold correctly)
  - ① Designed a wide variation of charges for a short peptide of 29 amino acid residues (~3600 Da).
    - 17 peptide sequences calculated, each with distinguished charges from -8, -7, -6, …, +6, +7, +8 (17 charge states).
    - 15 of the 17 sequences folded as desired (88% success rate).
    - 13 of the 18 exterior residues (72%) in the peptide were modified without disturbing the folded structures.
  - ② Designed a super-positive variant of human carbonic anhydrase II enzyme with net charge of +21 (natural enzyme has -1 charge).
    - This is the first example of a computationally designed super-positively charged enzyme.
    - 20 out of the enzyme's 70 exterior residues (28%) were mutated, without compromising the enzyme's folded structure or eliminating functionality (81% activity retained).
    - The super-positive enzyme variant can be directly encapsulated within a ferritin cage (negatively charged), without adding a super-positively charged fusion partner (previous encapsulation method).
    - The encapsulation leads to enhanced thermal stability and activity (63% enhanced at 40 °C).

- **Molecular dynamics (MD) simulations** (Uncovering unstable interactions in problematic sequences.)
  - For 2 sequences that did not fold correctly in synthesis, MD Simulations revealed unstable sidechain interactions near the peptides' N-terminus. MD supported redesigns which eliminated the found interactions folded correctly in experiments.

Undergraduate Researcher, University of Science and Technology of China **Jul 2014 – Jun 2016**

- Synthesized 3 microporous anion exchange membranes (crucial component of fuel cells) with exceptional high hydroxide conductivity and chemical stability. At the time of publication, one of the membranes demonstrated the highest conductivity at 80 °C reported in the field.

PUBLICATIONS

5 papers | 4 oral presentations | 10 + posters

1. **Guo, R.**; Sinha, N. J.; Misra, R..; Tang, Y.; Langenstein, M.; Kim, K.; Fagan, J. A.; Kloxin, C. J.; Jensen, G. V.; Pochan, D. J.; Saven, J. G., "Computational Design of Homotetrameric Peptide Bundle Variants Spanning a Wide Range of Charge States", *Biomacromolecules* 2022, 23, 4, 1652–1661
2. Sinha, N. J.; **Guo, R.**; Misra, R.; Fagan, J.; Faraone, A.; Kloxin, C. J.; Saven, J. G.; Jensen, G. V.; Pochan, D. J., "Colloid-Like Solution Behavior of Computationally Designed Coiled Coil Bundlemers" *Journal of Colloid and Interface Science*, 606 (2022) 1974–1982
3. Bulos, J. A.; **Guo, R.**; Wang, Z.; Delessio, M. A.; Saven, J. G.; Dmochowski, I. J., "Design of a Superpositively Charged Enzyme: Human Carbonic Anhydrase II Variant with Ferritin Encapsulation and Immobilization" *Biochemistry,* 2021, 60, 47, 3596–3609
4. *Yang, Z.; ***Guo, R.**; Malpass-Evans, R.; Carta, M.; McKeown, N. B.; Guiver, M. D.; Wu, L.; Xu, T., "Highly Conductive Anion-Exchange Membranes from Microporous Tröger's Base Polymers" *Angew. Chem. Int. Ed.* 2016, 55, 11499 –11502 [*co-first authors]
5. Yang, Z.; Liu, Y.; **Guo, R.**; Hou, J.; Wu, L.; Xu, T., "Highly Hydroxide Conductive Ionomers with Fullerene Functionalities" *Chem. Commun.*, 2016, 52, 2788-2791
6. **Guo, R.** et. al.; "Computational Design of The Electrostatic Features of Polymer-forming Peptide Bundles" *ACS Srping 2023 talk*

LEADERSHIP, TEACHING AND OUTREACH EXPERIENCE

Computational Lab Manager, Saven Lab **2018 –2023**

- Mentored 4 graduate students in research knowledge & tools, including protein design principles & algorithms; the group developed C++ code base; protein visualization & MD simulation software.
- Administrator of the group's Red Hat Linux based high-performance computing clusters and RAID arrays.

XSEDE Supercomputer Resource Proposal Manager, Saven Lab **2019 – 2023**

- Organizer and main contributor to the group's annual proposal for the Extreme Science and Engineering Discovery Environment (XSEDE) supercomputing resource allocation.
- Requests granted rate: 90% for 2022, 100% for 2021 & 2020, averaging ~70K CPU & 600K GPU node hrs.

Graduate Teaching Assistant, UPenn **Fall 2016 – Spring 2017 & Fall 2019 – Spring 2020**

- Rewarded "Commendation for Excellence in Teaching" in 2017 (8 awarded out of 32 TA candidates).
- Teaching courses include General Chemistry I, General Chemistry Lab I & II.

Philadelphia Area Girls Enjoying Science (PAGES) Outreach **Nov 2019**

- Contributed to the lecture design and instructed 60+ sixth-grade girls in the outreach, offering them hands-on experiences with science and fostering awareness of scientific career opportunities for women.

Vice Chairman of the Chemistry Student Group, School of Chemistry & Material Science, USTC **2014 – 2015**

- Leader of the technical department, producing posters (~20/year) and media contents for publicity purposes.