CURRICULUM VITAE

Payam Kelich

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EDUCATION

[01/2020-12/2023] **The University of Texas at El Paso, El Paso, TX**
Ph.D. Chemistry (expected graduation date: December 2023)
Dissertation: "Computation-Assisted Molecular Discovery for Biomedical Applications: Seeking Small Molecules and DNA Sequences with High Affinity Target Binding"
Supervisor: Dr. Lela Vuković

[09/2013-06/2016] **The Isfahan University of Technology, Isfahan, Iran**
Master's Degree, Polymer Engineering- Polymer Industry
Dissertation: "Molecular Dynamics Simulation of Poly (ethylene succinate) Crystallization Induced by Carbon Nanotubes and Graphene Nanosheets"
Supervisor: Dr. Ahmad Asadinezhad

[09/2008-09/2013] **The Isfahan University of Technology, Isfahan, Iran**
Bachelor's Degree. Chemical Engineering

WORK EXPERIENCES

[2024 - Present] **Postdoctoral Research Associate**
University of Illinois Urbana-Champaign, IL, USA
Supervisor: Dr. Emad Tajkhorshid
Responsibilities:

- Facilitating future research proposals by creating comprehensive preliminary data reports and project specifications, thereby improving team efficiency.
- Developing and maintaining the Linux infrastructure necessary for running molecular dynamics simulations and machine learning projects, enhancing research capabilities and outcomes.
- Conducting molecular dynamics simulations and applying machine learning techniques on membrane proteins to explore their dynamics and interactions, furthering the understanding of their biological functions.
- Engaging in the development and customization of VMD (Visual Molecular Dynamics) plugins to enhance visualization and analysis capabilities for molecular dynamics studies.

[2020 - 2024] **Ph.D. Research Associate**
University of Texas at El Paso, TX, USA
Supervisor: Dr. Lela Vuković
Responsibilities:

- Played an instrumental role in groundbreaking research concerning the binding and sensing of molecular analytes in DNA-CNT conjugates, driving forward the scientific understanding in this field.
- Facilitated future research proposals by creating comprehensive preliminary data reports and project specifications, thereby improving team efficiency.
- Participated in critical research of peptidomimetics, derived from genetically encoded libraries, for high-affinity binding to protein targets, contributing to advancements in drug design and biotechnology.

- Collaborated with international researchers to perform advanced computational modeling of nanoscale systems, promoting interdisciplinary knowledge exchange and expediting progress in nanotechnology research.
- Developed the Linux infrastructure necessary for running molecular dynamics (MD) simulations and machine learning projects, enhancing research capabilities and outcomes.

[2020-2024] **Ph.D. Teaching Assistant**
University of Texas at El Paso, TX, USA
- Assisted in delivering course materials for General Chemistry and Organic Chemistry labs, enriching the student's learning experience.

[2016 - 2019] **Python Programmer and DevOps Engineer**
Fanava IDC, Tehran, Iran
Responsibilities:
- Developed and implemented efficient Python scripts, streamlining business processes and data operations.
- Operated as a System Administrator for Linux servers, ensuring optimal performance, and security, and maintaining high uptime.
- Engineered, deployed, and maintained Python applications on Linux servers to enhance system efficiency and functionality.
- Worked as a Junior MLOps engineer, integrating Machine Learning models into production and managing the lifecycle of these models to ensure their effectiveness.

OTHER EXPERIENCES

[Jul 2024] **Advanced Python Instructor**
University of Maryland Institute for Health Computing, MD, USA
- Serving as an instructor for a summer school program on Pandas, a Python library for data manipulation and analysis.

PUBLICATIONS

Published Papers:

1. "Local Solvation of DNA Functionalized Carbon Nanotube Biosensors Probed with THz Spectroscopy". S.S. Nalige, P. Galonska, **P. Kelich**, S. Ramos, L. Sistemich, C. Herrmann, L. Vuković, S. Kruss, M. Havenith. *Nature Communication (accepted)*

2. "Predicting Serotonin Detection with DNA-Carbon Nanotube Sensors Across Multiple Spectral Wavelengths." **P Kelich**, J Adams, S Jeong, N Navarro, MP Landry, L Vukovic. *Journal of Chemical Information and Modeling*.
DOI: https://doi.org/10.1021/acs.jcim.4c00021

3. "Directed Evolution of Near-Infrared Serotonin Nanosensors with Machine Learning-Based Screening."S An, Y Suh, **P Kelich**, D Lee, L Vukovic, S Jeong. *Nanomaterials* 14,3 (2024).
DOI: https://doi.org/10.3390/nano14030247

4. "Genetically-Encoded Discovery of Perfluoroaryl-Macrocycles that Bind to Albumin and Exhibit Extended Circulation in-vivo". J.YK. Wong, A.I. Ekanayake, S. Kharchenko, S.E. Kirberger, R. Qiu, **P. Kelich**, S. Sarkar, E.R. Alvizo-Paez, J. Miao, S. Kalhor-Monfared, J.J. Dwyer, J.M. Nuss, Y.S. Lin, M.S. Macauley, L. Vuković, W.CK. Pomerantz, R. Derda. *Nature Communication* 14,1 (2023).
DOI: https://doi.org/10.1038/s41467-023-41427-y

5. "BinderSpace: A Package for Sequence Space Analyses for Datasets of Affinity-Selected Oligonucleotides and Peptide-Based Molecules" **P. Kelich**, H. Zhao, L. Vuković. *Journal of Computational Chemistry* (2023).

DOI: https://doi.org/10.1002/jcc.27130

6. "Characterizing the Interactions of Cell Membrane-Disrupting Peptides with Lipid-Functionalized Single-Walled Carbon Nanotube Systems for Antimicrobial Discovery" A. Yadav, **P. Kelich***, N.E. Kallmyer, N.F. Reuel, L. Vuković. *ACS Applied Materials & Interfaces,* 15, 24084–24096 (2023). (* co-first author)
DOI: https://doi.org/10.1021/acsami.3c01217

7. "Machine learning enables discovery of DNA-carbon nanotube sensors for serotonin". **P. Kelich**, S. Jeong, N. Navarro, J. Adams, X. Sun, H. Zhao, M.P. Landry, L. Vuković. *ACS Nano*, 16, 736–745 (2021).
DOI: https://doi.org/10.1021/acsnano.1c08271

8. "Computational Modeling of the Virucidal Inhibition Mechanism for Broad-Spectrum Antiviral Nanoparticles and HPV16 Capsid Segments". P. Chaturvedi, **P. Kelich**, T.A. Nikita, L. Vuković. *The Journal of Physical Chemistry B 125, 48, 13122–13131*(2021).
DOI: https://doi.org/10.1021/acs.jpcb.1c07436

9. "Genetically Encoded Fragment-Based Discovery from Phage-Displayed Macrocyclic Libraries with Genetically Encoded Unnatural Pharmacophores". A.I. Ekanayake, L. Sobze, **P. Kelich**, J. Youk, N.J. Bennett, R. Mukherjee, A. Bhardwaj, F. Wuest, L. Vuković, R. Derda. *Journal of the American Chemical Society,* 143, 5497–5507 (2021).
DOI: https://doi.org/10.1021/jacs.1c01186

10. "Molecular simulation study on brushes of poly (2-ethyl-2-oxazoline)", **P. Kelich**, A. Asadinezhad. *Materials Today Communications.* 21,100681(2019).
DOI: https://doi.org/10.1016/j.mtcomm.2019.100681

11. "Effects of carbon nanofiller characteristics on PTT chain conformation and dynamics: A computational study A. Asadinezhad, **P. Kelich**. *Applied Surface Science,* 392,981-990(2017).
DOI: https://doi.org/10.1016/j.apsusc.2016.09.137

12. "Adsorption of poly(ethylene succinate) chain onto graphene nanosheets: A molecular simulation", **P. Kelich**, A. Asadinezhad. *Journal of Molecular Graphics and Modelling,*69,26-38 (2016).
DOI: https://doi.org/10.1016/j.jmgm.2016.08.003

13. "Molecular Dynamics Insights into Behavior of Poly(ethylene succinate) Single Chain on Carbon Nanotube Surface", **P. Kelich**, A. Asadinezhad. *The Journal of Physical Chemistry C*, 119,26143-26153 (2015).
DOI: https://doi.org/10.1021/acs.jpcc.5b07844

Papers in preparation:

14. "Discovery of DNA-Carbon Nanotube Sensors for Oxytocin Detection Through Machine Learning, Generative Models, and Near-Infrared Fluorescence Spectroscopy". **P. Kelich**, J. Adams, M.P. Landry, L. Vuković.

15. "Machine Learning Models for Predicting the Subcellular Localization of Small Molecules". **P. Kelich**, A. Yadav, Md Nurunnabi, L. Vuković.

SKILLS

- **Major skills:** Machine learning, Data science, Cheminformatics, Molecular dynamics simulation, Molecular docking, Data mining, Database management, Generative AI.
- **Programming Languages:** Python, C, Bash Script, TCL
- **Python Machine Learning Libraries:** NumPy, Pandas, PyTorch, TensorFlow, Scikit-Learn, Deepchem, Matplotlib
- **Python Cheminformatics Libraries:** Biopython, RDKit
- **Computational Chemistry Software:** NAMD, AutoDock, VMD, MOE, Schrodinger Maestro, MDAnalysis
- **Operating Systems:** Linux, Unix-based operating systems, Docker

CERTIFICATES

[2023] Coursera: Machine Learning Specialization
[2023] Coursera: Deep Learning Specialization
[2023] Coursera: Generative Adversarial Networks (GANs) Specialization

PRESENTATIONS

[2021] Selected as a Texas Researcher to Present at TACC Symposium
P. Kelich, S. Jeong, N. Navarro, J. Adams, X. Sun, H. Zhao, M.P. Landry, L. Vuković, "Learning and Predicting DNA Sequences in DNA-nanotube Conjugates with High Response to Serotonin". *TACCSTER 2021 Proceedings,* Virtual meeting, 2021. (Presentation).

[2022] Presented at ACS Fall 2022 conference.
P. Kelich, S. Jeong, N. Navarro, J. Adams, X. Sun, H. Zhao, M.P. Landry, L. Vuković, "Machine learning and near-infrared fluorescence spectroscopy for discovery of DNA-carbon nanotube sensors of serotonin". *American Chemical Society Meeting*, Chicago, Illinois, August 21 - 25, 2022. (Presentation).

[2023] Presented at Annual Biochemistry and Chemistry Day at University of Texas at El Paso.
P. Kelich, What ChatGPT means for chemistry? concerns and ethical usage. (Presentation)

[2023] Presenting at ACS Fall 2023 conference.
P. Kelich, H. Zhao, L. Vuković, "BinderSpace: A Package for Sequence Space Analyses for Datasets of Affinity-Selected Oligonucleotides and Peptide-Based Molecules". *American Chemical Society Meeting*, San Francisco, California, August 13-17, 2023. (Poster).

[2023] Presenting at Theoretical and Computational Biophysics Group at UIUC.
P. Kelich.
"Computation-Assisted Molecular Discovery for Biomedical Applications: Seeking Small Molecules and DNA Sequences with High Affinity Target Binding"

[2023] Presenting at Ding Group at Tufts UTufts University.
P. Kelich.
"Computation-Assisted Molecular Discovery for Biomedical Applications: Seeking Small Molecules and DNA Sequences with High Affinity Target Binding"

MEDIA COVERAGE

[2021] Texas Advanced Computing Center highlighted our research. News Link
[2021] UTEP NewsFeed highlighted our NSF grant. News Link

LANGUAGE SKILLS

- **English**: Fluent
- **French:** Basic
- **Farsi** (Persian): Native

SERVICE

American Chemical Society (Since 2022)

Dr Vuković lab system admin (Since 2020)

REFERENCES

Dr. Lela Vuković, Associate Professor of Chemistry
Department of Chemistry and Biochemistry, The University of Texas at El Paso, El Paso, TX, USA.
Email: lVuković@utep.edu

Dr. Markita Landry, Associate Professor of Chemical and Biomolecular Engineering
Department of Chemical Engineering, the University of California, Berkeley, Berkeley, CA, USA.
Email: landry@berkeley.edu

Dr. Ratmir Derda, Professor of Chemistry
Department of Chemistry, the University of Alberta, Edmonton, AB, Canada.
Email: ratmir@ualberta.ca