

# CURRICULUM VITAE

## Payam Kelich

Email: [payam.kelich68@gmail.com](mailto:payam.kelich68@gmail.com)

Phone: +1 (915) 319-8752

Website: [payamkelich.github.io](https://payamkelich.github.io)

Visa status: Green Card Holder

### 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. "Fluorescence changes in carbon nanotube sensors correlate with THz absorption of hydration". S.S. Nalige, P. Galonska, **P. Kelich**, S. Ramos, L. Sistemich, C. Herrmann, L. Vuković, S. Kruss, M. Havenith. *Nature Communication* 15,1 (2024).  
DOI: <https://doi.org/10.1038/s41467-024-50968-9>
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*. 64, 10, 3992–4001(2024)  
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.jpcc.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 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: [lvukovic@utep.edu](mailto:lvukovic@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](mailto:landry@berkeley.edu)

**Dr. Ratmir Derda, Professor of Chemistry**

Department of Chemistry, the University of Alberta, Edmonton, AB, Canada.

Email: [ratmir@ualberta.ca](mailto:ratmir@ualberta.ca)