# Robert H. Lavroff

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### **EDUCATION**

University of California, Los Angeles Los Angeles, CA PhD Theoretical and Computational Chemistry Expected Graduation June 2025 Grade Point Average: 4.0 Relevant Coursework: Machine Learning Algorithms, Quantum Chemistry I & II, Statistical Mechanics, Computational Methods for Chemists, Methods of Materials Chemistry, Methods of Physical Chemistry, Solid State Physics (audit)

### Northwestern University

B.S. Chemical Engineering, Concentration in Environmental Engineering and Sustainability Graduated June 2018 Grade Point Average: 3.59 Chemistry Grade Point Average: 3.87 Relevant Coursework: Inorganic, Green, Physical, and Analytical Chemistry, Process Economics and Design, Probability and Statistics, Linear and Nonlinear Optimization

## **TECHNICAL SKILLS**

· Programming Languages: Python (with PyTorch, TensorFlow, RDKit, NumPy, sklearn, and PyMol), Bash, MUMPS (M), C#/.NET, TypeScript, SQL, HTML, CSS, Matlab, Mathematica

- · Additional Computer Programs: VASP, Gaussian, Aspen HYSYS, GAMS, ChemDraw, AutoCad, Microsoft Excel
- · Spectroscopy Experience: NMR (proton, C13, tungsten), UV-Vis, XRD, FT-IR, ATR-IR, BET, mass spectrometry

### **EXPERIENCE**

# Graduate Student Researcher, Department of Chemistry

Alexandrova Research Group, University of California, Los Angeles, Los Angeles, CA

- · Develop software and implement machine learning algorithms to predict chemical reactivity and design new
- heterogeneous catalysts and nanoparticles using spectroscopic and energetic data
- · Perform optimization and electronic calculations to study formation of metal oxide fractals on gold surfaces
- Study the effects of applied electric fields on metal surfaces to tune catalytic activity in industrial reactions

## Rotational Student Researcher, Department of Chemistry

Houk Research Group, University of California, Los Angeles, Los Angeles, CA

- · Performed transition state and intrinsic reaction coordinate calculations in Gaussian to determine mechanism of
- kinetically controllable Pd-catalyzed decarboxylation enabled [5+2] and [3+2] cycloaddition toward carbocycles · Academic paper submitted for publication

## Technical Solutions Engineer, Inpatient Pharmacy Application

Epic Systems, Verona, WI

· Completed 23 software development projects improving environment management and pharmacy functionality, including front-end user interface creation and Intersystems Cache data manipulation

· Managed a group of twenty technical solutions engineers as PeaceHealth's Epic Technical Coordinator, hosting weekly calls with hospital executives and mobilizing quarterly software upgrades onto servers and clients

- Taught a two hour course on web development and debugging to an audience of approximately 150 coworkers
- · Managed hospital escalations by coordinating tailored development projects with Epic software developers
- · Provided project management and advisory services to Cleveland Clinic, Hurley Medical Center, and United Regional Healthcare System on pharmacy electronic medical software, including code debugs, user coaching, and upgrade support

· Managed an internal workgroup of fifteen people focused on interfacing with third-party hardware, with emphasis on patient care and reporting reliability

· Mentored new technical solutions engineers throughout their first year at Epic

October 2020-January 2021

August 2020-Present

July 2018-July 2020

Evanston, IL

# Summer Co-Op, Central Project Management Division

Bayway Refinery, Infineum International, Linden, NJ

- · Planned and coordinated three global dispersant manufacturing projects valued between \$400,000 and \$50 million
- · Summarized and evaluated project scheduling and safety trends for future improvement of annual plant operations
- · Presented and defended accomplishments throughout the co-op at a company-wide final presentation

# Research Assistant, Department of Chemistry

Hupp Research Group, Northwestern University, Evanston, IL

- · Synthesized and tested zirconium-based metal-organic framework catalysts for oxidative disarming of mustard gas
- · Spectroscopically characterized frameworks via BET and NMR
  - · Academic paper published in the American Chemical Society's Journal of Applied Materials and Interfaces

# **Research Assistant and Developer, Department of Chemistry and Chemical Biology** January 2015-June 2018

Lawrence Williams Research Group, Rutgers Chemistry, Piscataway, NJ

- $\cdot$  Developed iterative algorithms to model and predict the folding of chains of 13-120 amino acids using statistical thermodynamics
- $\cdot$  Studied effects of protein mutations on formation of secondary structure
- · Academic paper published in TECHNOLOGY Journal Vol 07, No. 01n02

# Summer REU Intern, Department of Chemical Engineering

Christopher Williams Research Group, University of South Carolina, Columbia, SC

- · Developed four economical and sustainable SiO2 catalysts for conversion of syn gas into ethylene glycol
- $\cdot$  Analyzed in-situ FT-IR spectra to quantify catalyst stability and selectivity
- · Presented research at AIChE National Conference Student Poster Session in San Francisco

# Research Assistant, Department of Chemical Engineering

You Research Group, Northwestern University, Evanston, IL

- · Leveraged nonlinear and nonconvex optimization to determine efficient feedstock ratios for shale gas generation
- · Generated complex chemical process system simulations for these reactions in Aspen HYSYS
- · Analyzed shale gas feedstock from various geographical locations for realistic simulation

# Aresty Research Scholar, Department of Chemical and Biochemical EngineeringMay 2015-September 2015Celik Catalysis Group, Aresty Research Center, Piscataway, NJMay 2015-September 2015

- · Developed and tested TiO<sub>2</sub>-based photocatalysts for the conversion of CO<sub>2</sub>-fixing biomass to hydrogen fuel
- · Worked up and analyzed catalytic reaction data using UV-Vis spectroscopy
- · Full time summer research position, 40 hours per week

# **Research Assistant and Developer, Department of Materials Science and Engineering** January 2015-May 2015 *Birnie Research Group*, **Rutgers Engineering**, Piscataway, NJ

- · Synthesized and analyzed dye-sensitized solar cells and polymer-solenoid harmonic systems
- $\cdot$  Computer modeling of distance-dependent Fickian diffusivity

# **PUBLICATIONS**

Improving the Efficiency of Mustard Gas Simulant Detoxification by Tuning the Singlet Oxygen Quantum Yield in Metal–Organic Frameworks and Their Corresponding Thin Films

Cassandra T. Buru, Marek B. Majewski, Ashlee J. Howarth, Robert H. Lavroff, Chung-Wei Kung, Aaron W. Peters, Subhadip Goswami, and Omar K. Farha

ACS Applied Materials & Interfaces 2018 10 (28), 23802-23806

DOI: 10.1021/acsami.8b05792

June 2016-August 2016

January 2016-March 2016

September 2016-June 2017

June 2017-September 2017

# A protein interaction free energy model based on amino acid residue contributions: Assessment of point mutation stability of T4 lysozyme

Lawrence J. Williams, Brian J. Schendt, Zachary R. Fritz, Yonatan Attali, Robert H. Lavroff, and Martin L. Yarmush TECHNOLOGY 2019 07:01n02, 12-39 DOI: 10.1142/S233954781950002X

# Surface Spectroscopic Study of Renewable Ethylene Glycol Synthesis over Silicon Dioxide-Supported Metal Catalysts (*Poster Presentation*)

AIChE Annual Meeting, San Francisco, CA, November 2016 Robert Lavroff, Christopher Williams and Xinbin Yu, Chemical Engineering, University of South Carolina, Columbia, SC

# Production of Hydrogen via Visible-Light Photocatalytic Methane Steam Reforming Over Modified Titanium Dioxide (*Poster Presentation*)

Catalysis Club of Philadelphia Annual Student Poster Contest, Wilmington, DE, November 2015 A.M. Pennington, K.A. Dagnall, R.A. Yang, R.H. Lavroff, K.M. Dickson, F. E. Celik, Chemical and Biochemical Engineering, Rutgers University, New Brunswick, NJ

# INDEPENDENT SOFTWARE DEVELOPMENT PROJECTS

February 2018: Wrote a non-linear optimization program in GAMS which takes in the movie preferences of a group of people and provides a "movie marathon" recommendation list using IMDB data

December 2017: Created a machine learning (principal component analysis and linear discriminant analysis) model in Matlab, and Visual Basic for insight on Florida presidential results

### LEADERSHIP & EXTRACURRICULARS

Program for Excellence in Education Research in the Sciences (PEERS) Facilitator September 2020 - Present

- · Tutor groups of five to thirty students from underrepresented and under-served populations
- · Facilitate remote student success through collaborative learning (CL) strategies
- · Multiple quarters of experience tutoring general and organic chemistry for both physical and life science students

### Tutoring, General and Organic Chemistry, Engineering Mechanics, Mathematics

- · Worked as a freelance organic chemistry tutor for three Northwestern students
- · Tutored freshman engineering courses through Engineering Office of Student Services

### Northwestern Ski and Snowboard Team, Public Relations and Alumni Chairman

- · Created quarterly newsletters and events for team alumni, managed team website and social media accounts
- · Coordinated weekly race logistics, maintaining regular communication with USCSA and MSCA officials

### Engineers Without Borders, Technical Team Member

- · Designed rain water filtration and collection system in AutoCad
- · Planned and coordinated March 2017 system installation in Kenyan village

### American Institute of Chemical Engineers, Professional Member

• Member of Process Development Division, Fuels and Petrochemicals Division, and Sustainable Engineering Forum

September 2014-June 2018

February 2018-Present

May 2016-June 2018

September 2014-June 2018