

EDUCATION

University of Houston - Houston, TX, US*Ph.D, Chemistry (GPA: 3.6)*

Anticipated graduation: MAY 2016

- Dissertation: *Ab initio* Calculations of Intramolecular Charge and Energy Transfer with Reduced Modes in Donor-bridge-acceptor Species
- Advisor: Dr. [Eric R. Bittner](#)

Xiamen University - Xiamen, Fujian, China*Bachelor of Science, Chemistry; Mathematics Minor*

JULY 2009

- Thesis: Study of Weak Interaction and Aromatic Carbon Atom in DREIDING Force Field

Udacity - [Machine Learning Nanodegree](#)

FEBRUARY 2016

Udacity - [Data Analyst Nanodegree](#)

SEPTEMBER 2015

SKILLS

Working knowledgePython, Mathematica, R, HTML/CSS, D3.js, Octave/MATLAB, SQL, TensorFlow, SAS, Vim, Linux, L^AT_EX, Q-Chem, Gaussian, various chemistry instruments**Basic knowledge**

JavaScript, MongoDB, Hadoop, HBase, Pig, Hive, Spark, Splunk, FORTRAN, C, Haskell

Languages

Fluent in English, Chinese. Proficient in Taiwanese.

PROJECT

[English Letter Recognition](#)

FEBRUARY 2016

EXPERIENCE

- Trained a 6 layer convolutional neural network with 95% accuracy on [notMNIST](#) dataset using TensorFlow

[Clustering of Vervet Monkey's Alarms](#)

FEBRUARY 2016

- Verified the classical discovery of three types of alarms in vervet monkey by hierarchical, k-means and partitioning around medoids (PAM) clustering, achieved at least 75% classification accuracy
- Built an AdaBoost model with 99% prediction accuracy

[Creating Customer Segments](#)

JANUARY 2016

- Applied PCA and independent component analysis (ICA) to a customer dataset of a wholesale distributor to preprocess and understand purchasing behavior better
- Used Gaussian mixture model to find customer segments for better A/B test on policy change

[Train a Smartcab to Drive](#)

JANUARY 2016

- Taught toy smartcab traffic laws and best routing strategy with Q-learning. The driving agent is able to consistently reach the destination within allotted time with 90% success rate

[Forum Data Analysis](#)

OCTOBER 2015

- Analyzed the posts on Udacity's forum using Hadoop MapReduce codes

[PISA Data Visualization](#)

SEPTEMBER 2015

- Explored the relations between family possessions and student scores in the Programme for International Student Assessment (PISA) data using R and Python
- Visualized the analysis with interactions using D3.js and dimple.js

Red Wine Study

SEPTEMBER 2015

- Modeled the influence of various chemicals to red wine quality on a wine [dataset](#) by linear regression with Lasso in RStudio

Increased-by-one Single Tape Turing Machine

JUNE 2015

- Implemented an increased-by-one single tape Turing machine program with only HTML/CSS, inspired by a [discussion](#) of the Turing completeness of HTML/CSS

Identifying Fraud from Enron Email

MAY 2015

- Investigated the Enron email corpus data with decision tree, Gaussian naive Bayesian, and k-means clustering machine learning techniques

Houston Map Data Wrangling

MAY 2015

- Cleaned the map data on [openstreetmap](#) of the great Houston area (file size > 500M)
- Analyzed the cleaned data with MongoDB queries

New York Subway Data Analysis

MAY 2015

- Statistically tested the relation between the ridership of subway and weather in New York

CERTIFICATES

SAS Certified Base Programmer for SAS 9 Credential

11 computer science courses on edX, Coursera and Udacity (certificates available on my [LinkedIn](#))**RESEARCH &
TEACHING
EXPERIENCE****University of Houston**, Houston, TX*Research & Teaching Assistant*

AUGUST 2010 - PRESENT

- Developed and coded in Mathematica a new theoretical molecular dynamics analysis scheme based on Lanczos algorithm and time-convolutionless master equation
- Benchmarked the scheme with a classical series of molecules and researched the dynamics
- Optimized the geometry of tripodal amine-Cu(I) complexes using density functional theory (DFT), to assist further research of their reactivity and stability
- Teach general and physical chemistry labs independently. Instruments used include UV/VIS, FT-IR, ESR, NMR, STM and XRD

Xiamen University, Xiamen, Fujian, China*Research Assistant*

AUGUST 2009 - JUNE 2010

- Implemented FORTRAN programs for the point group and atom type recognition in AMBER and DREIDING force fields, as part of efficient QM/MM method development

PUBLICATIONS**Intramolecular Charge and Energy Transfer Rates with Reduced Modes: Comparison to Marcus Theory for Donor-Bridge-Acceptor Systems**Yang, Xunmo and Bittner, Eric. *The Journal of Physical Chemistry A*, 2014, 118(28), pp 5196-5203**Computing Intramolecular Charge and Energy Transfer Rates using Optimal Modes**Yang, Xunmo and Bittner, Eric. *The Journal of Chemical Physics*, 142, 244114 (2015)**Tripodal Amine Ligands for Accelerating Cu-Catalyzed Azide-Alkyne Cycloaddition: Efficiency and Stability against Oxidation and Dissociation**Zhiling Zhu, Siheng Li, Haoqing Chen, Yongkai Huang, Xunmo Yang, Eric Bittner, and Chengzhi Cai. (Submitted to *Organic & Biomolecular Chemistry*)**PATENT****Coriolis force experiment plate**

No.: CN 2665845 Y

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