## Xunmo Yang

#### EDUCATION

#### University of Houston - Houston, TX, US

Ph.D, Chemistry (GPA: 3.6)

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 Engineer Nanodegree

FEBRUARY 2016

**Udacity** - Data Analyst Nanodegree

SEPTEMBER 2015

#### Work History

#### Google, Mountain View, CA

Software Engineer

JAN 2017 - PRESENT

- Analyze large scale data for better user experience in Ads

#### University of Houston, Houston, TX

Post Doctoral Fellow

SEPTEMBER 2016 - NOVEMBER 2016

- Identified electron transfer coordinates in Donor-Bridge-Acceptor systems using mode projection analysis

## University of Houston, Houston, TX

Research & Teaching Assistant

AUGUST 2010 - MAY 2016

- 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
- Taught general and physical chemistry labs independently. Instruments used include UV/VIS, FT-IR, ESR, NMR, STM and XRD

#### SKILLS

#### Working Knowledge

Python, Mathematica, R, HTML/CSS, D3.js, Octave/MATLAB, SQL, TensorFlow, SAS, Vim, Linux, ŁTFX, Q-Chem, Gaussian, various chemistry instruments

#### Basic Knowledge

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

#### Languages

Fluent in English, Chinese. Proficient in Taiwanese.

#### Project Experience

## Pseudo-hologram Video Maker

May 2016

- Deployed an OpenCV-based program online for pseudo-hologram video conversion using Flask

**English Letter Recognition** 

FEBRUARY 2016

- 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

#### Train a Smartcab to Drive

JANUARY 2016

- Taught toy smartcab traffic laws and best routing strategy with Q-learning. The driving agent was able to consistently reach the destination within allotted time with 95% 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

## 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

## 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

#### The Essential Hayek Translation

**MARCH 2016** 

Issued: 12/22/2004

- Translated *The Essential Hayek* voluntarily to Chinese

#### CERTIFICATES

## SAS Certified Base Programmer for SAS 9 Credential

11 computer science courses on edX, Coursera and Udacity (certificates available on my LinkedIn)

#### **Publications**

# Identifying electron transfer coordinates in donor-bridge-acceptor systems using mode projection analysis

Xunmo Yang, Theo Keane, Milan Delor, Anthony J. H. M. Meijer, Julia Weinstein & Eric R. Bittner. *Nature Communications*, **2017**, *8*, 14554

Intramolecular Charge and Energy Transfer Rates with Reduced Modes: Comparison to Marcus Theory for Donor-Bridge-Acceptor Systems

Xunmo Yang and Eric Bittner. The Journal of Physical Chemistry A, 2014, 118(28), pp 5196-5203

Computing Intramolecular Charge and Energy Transfer Rates using Optimal Modes Xunmo Yang and Eric Bittner. *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, Haoqing Chen, Siheng Li, Xunmo Yang, Eric Bittner, Chengzhi Cai. *Catalysis Science* & Technology, 2017, 7, 2474-2485

No.: CN 2665845 Y

PATENT Coriolis force experiment plate