# Xunmo Yang

832-519-8420
xunmoyang@gmail.com
https://github.com/tcya
linkedin.com/in/xunmoyang

## 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 Engineer Nanodegree February 2016
**Udacity** - Data Analyst Nanodegree September 2015

## Skills

**Working Knowledge**
Python, Mathematica, R, HTML/CSS, D3.js, Octave/MATLAB, SQL, TensorFlow, SAS, Vim, Linux, LaTeX, 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 Experience

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

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 was 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

<The Essential Hayek> Translation — March 2016
- 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)

## 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
- Taught 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 — Issued: 12/22/2004