Xunmo Yang

https://github.com/tcya
linkedin.com/in/xunmoyang

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 of 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, LaTeX, 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
- 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

Patent

Coriolis force experiment plate — No.: CN 2665845 Y — Issued: 12/22/2004