Xunmo Yang

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

EDUCATION

Udacity - Data Analyst Nanodegree

SEPTEMBER 2015

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

SEPTEMBER 2005 - JULY 2009

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

Skills

Working knowledge

Python, Mathematica, R, HTML/CSS, D3.js, Octave, SQL, Vim, Linux, ŁTŁX, Q-Chem, Gaussian Basic knowledge

JavaScript, MongoDB, SAS, Hadoop, MATLAB, FORTRAN, C, various chemistry instruments

Languages

Fluent in English, Chinese and Taiwanese

Project Experience **Udacity** - Data Analyst Nanodegree

JANUARY - SEPTEMBER 2015

PISA Data Visualization

github.com/tcya/PISA-visualization

- 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

Identifying Fraud from Enron Email

github.com/tcya/Identify-Enron-Corporate-Fraud

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

Red Wine Study

github.com/tcya/what-affects-red-wine-quality

- Modeled the influence of various chemicals to red wine quality on a wine dataset by linear regression with Lasso

Houston Map Data Wrangling

github.com/tcya/houston-mapdata-wrangling

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

New York Subway Data Analysis

github.com/tcya/new-york-subway-data-analysis

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

A/B Testing

- Evaluated a hypothetical A/B test trying to reduce the number of frustrated students after enrollment on Udacity

Udacity - Intro to Hadoop and MapReduce

OCTOBER 2015

Forum Data Analysis

github.com/tcya/udacity-forum-hadoop-analysis

- Programmed some MapReduce codes for Hadoop to analyze the posts in Udacity's forum.

Independent Coursework Udacity: 6 computer science courses (certificates available on my LinkedIn) edX: 2 computer science courses (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

Issued: 12/22/2004

- 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

Zhu, Zhiling; Chen, Haoqing; Li, Siheng; Huang, Yongkai; Yang, Xunmo; Bittner, Eric; Cai, Chengzhi. (Submitted to *The Journal of Organic Chemistry*)

No.: CN 2665845 Y

Patent

Coriolis force experiment plate