Xunmo Yang

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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/MATLAB, SQL, 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 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)
Coursera: 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

- 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