DIEGO GOMEZ

New Orleans, LA

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RESEARCH INTERESTS

Applications: Statistical mechanics and thermodynamics of ionic solutions relevant to molecular biophysics, molecular simulation and design of electrical energy storage.

Methods: Using *quasi-chemical theory* (QCT) by sampling dynamic quantum mechanic/molecular mechanics (QM/MM) simulation through a variety of quantum chemistry software programs.

EDUCATION

B.S., New Mexico State University, Chemical Engineering, 2017

Ph.D., Tulane University, Chemical Engineering, 2021 (Expected)

POST UNDERGRADUATE EMPLOYMENT

Graduate Research Assistant, Tulane University, New Orleans, LA, 2017-Present

- Addressing the comparative behavior of the aqueous halides F^-, Cl^-, Br^-, and I^- on the basis of QCT. This work requires a variety of techniques through multiple quantum chemistry software suites taking advantage of high-performance computing (HPC) resources.
- Studying the structures and free energies of hydrated clusters for ions present in the desalination of processed water over a range of extreme temperatures (T) and pressures (p).
- Investigating physical properties of capillary bridges and completing the mathematical physics presented by Pierre-Gilles de Gennes.

HPC Research and Development Intern, Sandia National Laboratories, Livermore, CA, 2017

- Using HPC resources, ported a MATLAB classifier to a highly distributed program using Python and APACHE PySpark.
- Developed a technical document to help non-developer written programs using big data, quickly and easily take advantage of HPC resources using PySpark.

SKILLS

Research

- CP2K for bulk *ab-initio* molecular dynamics (AIMD) of solvated ions, and for gas-phase dynamics of hydrated ions.
- Geometry optimization and single-point energy calculations using Gaussian16.
- Statistical mechanics of molecular dynamics simulation using GROMACS.
- Installation and optimization of quantum chemistry packages on HPC resources.

AIMD | CP2K | Gaussian16 | HPC | GROMACS

Development

- R for data analysis and visualization including publication-quality figures.
- Python and R for machine learning applications.
- Scientific computations using HPC resources with C++ with MPI or OpenMP.
- Creation and implementation of SHELL scripts for Unix and *nix operating systems.

R | Python | C++ | MPI | OpenMP | Bash | C shell

Writing

- Using LaTeX for first-author publications, presentations, and technical documents.
- Using Wordpress for a personal blog related to the presentation of statistical mechanics related problems.

LaTeX | WordPress

UNDERGRADUATE EMPLOYMENT

Process Engineering Intern, Chevron Phillips Chemical Company, Borger, TX, 2016

Engineering Mentor, New Mexico State University, Las Cruces, NM, 2014-2017

Research Experience for Undergraduates, University of New Mexico, Albuquerque, NM, 2015

Undergraduate Researcher, New Mexico State University, Las Cruces, NM, 2013-2014

GRADUATE COURSEWORK

Chemical Engineering: Thermodynamics, Transport Phenomena, Reactor Design, Statistical Mechanics, Capillary Phenomena, Machine Learning.
Chemistry: Quantum Mechanics, Computational Quantum Chemistry.
Computer Science: C++ for Scientists and Engineers, Large Scale Computation Using C++, Machine Learning.
Mathematics: Stochastic Processes.

PROFESSIONAL AFFILIATIONS

American Institute of Chemical Engineers (AIChE)
Tulane University Graduate Studies Student Association (GSSA)

PRESENTATIONS

1. Department of Chemical Engineering, Tulane University, December 2018
2. Los Alamos Chemistry Division, Los Alamos National Laboratory, February 2020
3. Department of Chemical Engineering, Tulane University, April 2021

PUBLICATIONS

Articles

(*1*) Gomez, D. T., Pratt, L. R., Rogers, D. M., and Rempe, S. B. (2021). Free Energies of Hydrated Halide Anions: High Through-Put Computations on Clusters to Treat Rough Energy-Landscapes. *Molecules 26*, DOI: 10.3390/molecules26113087.