DANJO DE CHAVEZ

PhD, Chemical Sciences and Engineering
Molecular Chemistry and Engineering Specialization

@ danjo.dechavez@kemi.uu.se Uppsala, Sweden

WORK EXPERIENCE

Post-Doctoral Researcher
Department of Chemistry - BMC, Uppsala University
August 2022 - Present Uppsala, Sweden

I am working on machine learning based method development for multiconfigurational quantum chemistry applications in OpenMolcas.

Post-Doctoral Researcher
Institute for Catalysis, Hokkaido University
October 2021 - August 2022 Sapporo City, Japan

I developed computational tools and used quantum chemical simulation to elucidate chemical reaction under external mechanical stress.

Research Assistant
Institute for Catalysis, Hokkaido University
July 2021 - September 2021 Sapporo City, Japan

I studied mechanochemical reactions using my original Python code interfaced with other quantum chemical software.

Teaching Assistant
College of Science, Hokkaido University
October 2019 - March 2020 Sapporo City, Japan

I was a lecture assistant for catalytic chemistry and computational chemistry courses.

Instructor 1
Institute of Chemistry, University of the Philippines Diliman
June 2012 - April 2016 Quezon City, Philippines

I also have experience in teaching various undergraduate laboratories such as biochemistry, analytical and organic chemistry.

EDUCATION

PhD Chemical Sciences and Engineering
Hokkaido University
October 2018 - September 2021 Sapporo, Hokkaido, Japan

MSc Chemical Sciences and Engineering
Hokkaido University
October 2016 - September 2018 Sapporo, Hokkaido, Japan

BS Biochemistry
University of the Philippines Manila
June 2008 - April 2012 Manila, Philippines

RESEARCH INTERESTS

- Biomolecular Simulations and Informatics
- Computational and Theoretical Chemistry
- Data Mining and Machine Learning

TECHNICAL SKILLS

Programming Languages

Python	●●●●○
R	●●●○○
FORTRAN	●●●○○
C++	●●●○○
Bash	●●●●○

Chemical Softwares

- Gaussian
- Siesta
- ORCA
- DC-DFTBK
- GROMACS
- NAMD
- AMBER
- Discovery Studio

STRENGTHS

- Hard-working
- Research
- Programming
- Critical Thinking
- Problem Solving
- Teamwork
- Resiliency

LANGUAGES

English	●●●●●
Tagalog	●●●●●
Japanese	●●●○○

WORKSHOP AND SPECIALIZATIONS

Python 3 Programming Specialization
University of Michigan

May 2020 | Coursera

- Python Basics
- Python Functions, Files, and Dictionaries
- Data Collection and Processing with Python
- Python Classes and Inheritance
- Python Project: pillow, tesseract, and opencv

TensorFlow in Practice Specialization
deeplearning.ai

February 2020 | Coursera

- Introduction to TensorFlow for Artificial Intelligence, Machine Learning, and Deep Learning
- Convolutional Neural Networks in TensorFlow
- Natural Language Processing in TensorFlow
- Sequences, Time Series and Prediction

Open Source Software Development, Linux and Git Specialization
The Linux Foundation

January 2019 | Coursera

- Open Source Software Development Methods
- Linux for Developers
- Linux Tools for Developers
- Using Git for Distributed Development

5th Asian Computational Materials Design Workshop (ACMD)
Material Simulations and Design

2012 | Manila, Philippines

Introduction to Computational Chemistry and Application
First Principles Calculations and Monte Carlo Simulations

2012 | Quezon City, Philippines

SCHOLARSHIPS AND RECOGNITION

Japanese Government (Monbukagakusho) Scholarship
Hokkaido University

April 2016 - September 2021 | Sapporo, Hokkaido, Japan

- Doctor of Philosophy Program
- Master's Degree Program
- Research Studentship

Best Undergraduate Research (Candidate)
BSc in Biochemistry,
University of the Philippines - Manila

April 2012 | Manila, Philippines

ORGANIZATIONS

Hokkaido University Association of Filipino Students
April 2016 - Present

Integrated Chemists of the Philippines
September 2012 – Present

Philippine Association of Chemistry Students
2009 – 2012

UP Biochemistry Society
2009 – 2012

VOLUNTEER WORK

Project Kapnayan
Institute of Chemistry,
University of the Philippines

2012-2016

Project Kapnayan is the official extension arm of the Institute of Chemistry promoting chemistry to high school students.

UP Pahinungod
University of the Philippines

2013-2015

Pahinungod is the official extension social civic arm of the University of the Philippines.

UP Learning Resource Center Tutor
University of the Philippines

2010-2012 | Manila, Philippines

Peer tutor for Chemistry, Physics and Mathematics

REFERENCES

Prof. Jun-ya Hasegawa
Hokkaido University
hasegawa@cat.hokudai.ac.jp

Assoc. Prof. Kenji Iida
Hokkaido University
k-iida@cat.hokudai.ac.jp

Prof. Junie Billones
University of the Philippines
jbbillones@up.edu.ph

SUMMARY OF PAST AND CURRENT RESEARCH

Theoretical Studies on Mechanocatalytic Systems

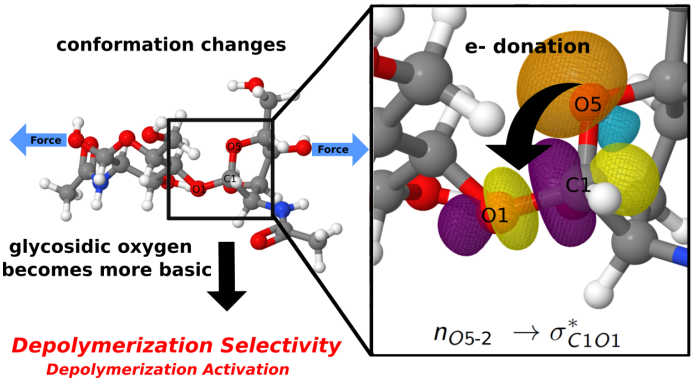
Hokkaido University

Ongoing

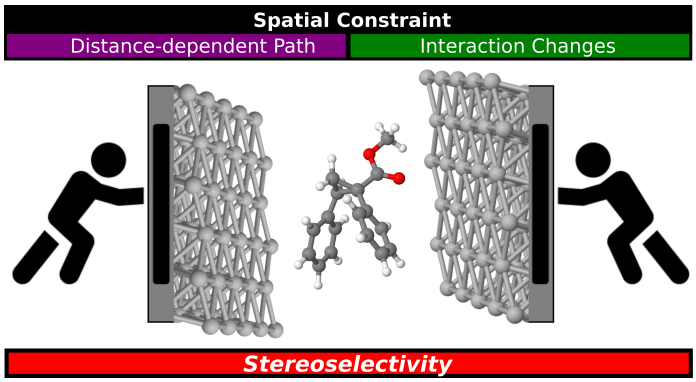
This is a thematic research project revolving around mechanochemistry with applications to catalysis. It is comprised of 3 projects which aimed to sample the effect of mechanical forces on reactants, transition states as well as catalysts. This serves as my dissertation for the degree PhD in Chemical Science and Engineering. Mechanochemistry provides a unique activation mode with the use of force vectors with which novel applications have been developed.

- **On the Electronic Structure Origin of Mechanochemically Induced Selectivity in Acid Catalyzed Chitin Hydrolysis**

  In this part, I studied the mechanochemical effect of pulling on chemical reactivity. I developed a code that employs the FMPES (Force Modified Potential Energy Surface) formalism in the G09 package. This code includes an user defined external pulling force during simulations. After code development, the reaction mechanisms and pulling simulations were done in both reactant and transition state. It was found that during pulling, the glycosidic oxygen becomes more basic and hence more susceptible to acid catalysis. This work was chosen as a supplementary cover for the Journal of Physical Chemistry A.



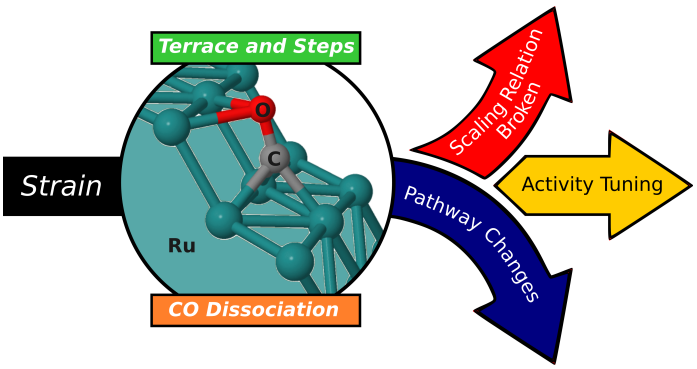
- **Mechanical Pushing Induced Selective Cyclopropanation Reaction in Ag(111) Surface**



  This work employs DFT (Density Functional Theory) calculation to determine the mechanical effect in a selective cyclopropanation reaction. In this study, a metal sandwich model was devised to mimic the reaction environment. Also, the mechanical pushing effect was taken into account with a decrease in the slab distances. This offers a unique constraining environment for the reaction center. Preliminary results show that a single slab (corresponding to a relaxed system) shows a different selectivity observed experimentally, revealing that mechanical constraint is needed. It also attests that there is a distance-dependent pathway preference for the reaction. This work emphasizes the capability of mechanical forces to change the reaction mechanism as well as to dictate selectivity.

- **Potential of Compressive Strain in Increasing Catalytic Activity of Ru in CO Decomposition**

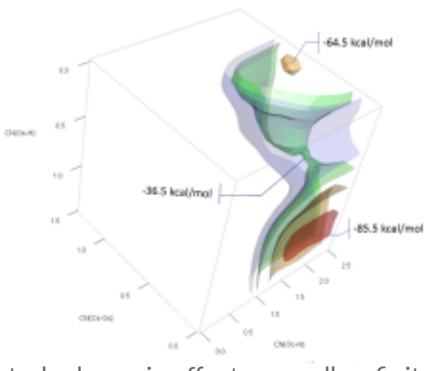
  In this system, the effect of isotropic and anisotropic strain in a catalytic surface is being studied. Specifically, the CO decomposition activity of relaxed and strained Ru(0001) and Ru(1015) surfaces was investigated. Adsorption-Strain relations have been analyzed using the conventional d-band model as well as the novel Eigenstress model. Reaction pathways were studied using NEB calculations to determine the transition state. This revealed pathways with a lower activation barrier which was expected from the traditional Bronsted-Evans-Polyani (BEP) relation. However, cases in which the BEP relationship was broken which can lead to higher catalytic activity was also found. This work opens another method to break scaling relation in heterogenous catalysis and to tune its catalytic activity.

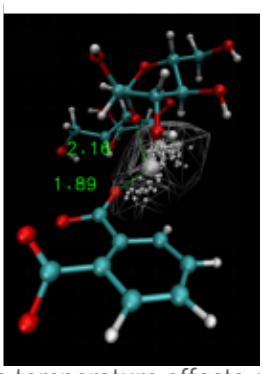


Role of Vicinal H bonding Groups to Organic Acid Catalyzed Glucan Hydrolysis

Hokkaido University

2018-2019





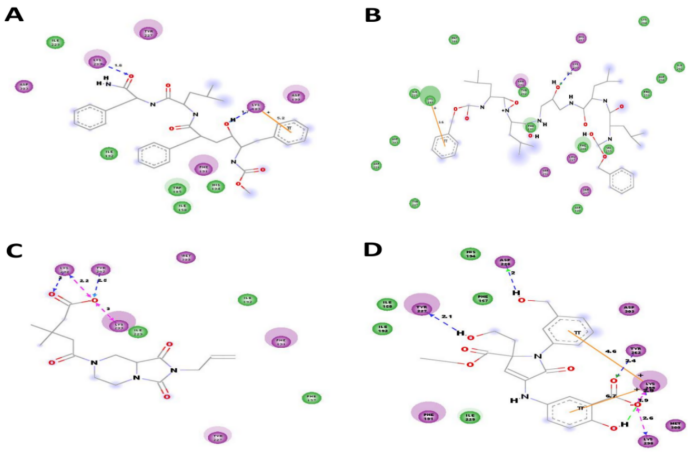
In this work, we studied the effect of hydrogen bonding moieties of acid catalysts in glucan hydrolysis. Benzoic acid and its derivatives served as model catalysts to mimic the character of oxidized activated carbon which was found to have acidic groups. Our initial study of glucan interaction with the model catalysts found that the stability of the complex is directly related to the catalytic activity in experiments. We further analyze the potential energy surface of the reactions and found that protonated system closely modeled the experimental activation energy. This suggested cooperation with the previously dissolved proton and the catalyst. To study dynamic effects as well as finite temperature effects, we utilized Density Functional Theory Binding Metadynamics. Metadynamics is a biased sampling technique which hastens the simulation of rare events such as proton transfer reactions. This elucidated that the neighboring h-bonding group orients a solvated proton to the active site facilitating cleavage.

Structure-Based Pharmacophore Generation and Virtual Screening of Possible Inhibitors of Homology Modeled Plasmodium falciparum Signal Peptide Peptidase

University of the Philippines Manila

2011-2012

Malaria parasites include five plasmodium species specifically *Plasmodium falciparum*, *P.vivax*, *P.ovale*, *P. malariae P. knowlesi* which are present in the Philippines. Recently, there is a growing resistance to anti-malarial drugs hence the need for the development of new therapeutics against malaria. *Plasmodium falciparum* Signal Peptide Peptidase (PfSPP) is a conserved protein sequence in all five species and served as drug target. Three-dimensional structure of PfSPP was generated via homology modelling and was used to generate a pharmacophore model, which was subsequently used to screen over 170,000 library compounds. At the end of the work, 3 compound leads were found bind better than a known drug which renders them as lead compounds. The high-scoring compounds were docked to the target enzyme and the high affinity hits were further developed in silico using De Novo Evolution technique. After which, lead compounds further increased their binding to the active site. This work served as my undergraduate thesis and was selected as one of the best biochemistry thesis in 2012.

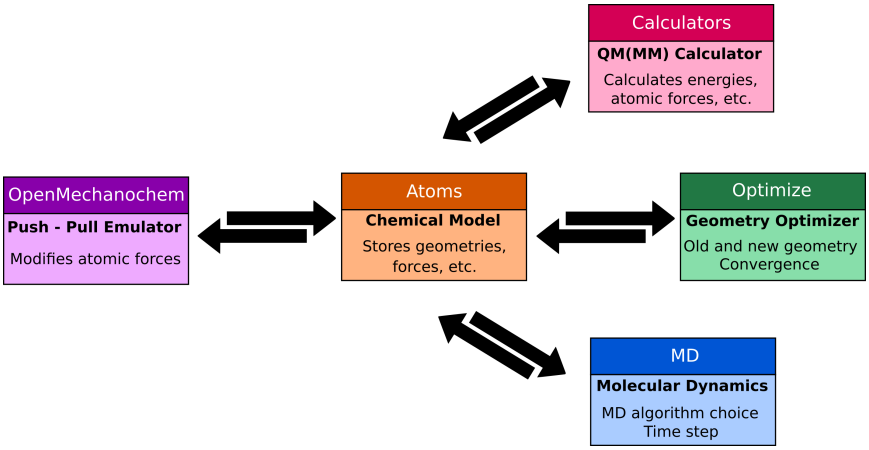


GIT, PYPI, AND DEVELOPMENT EXPERIENCES

OpenMechanochem

Hokkaido University

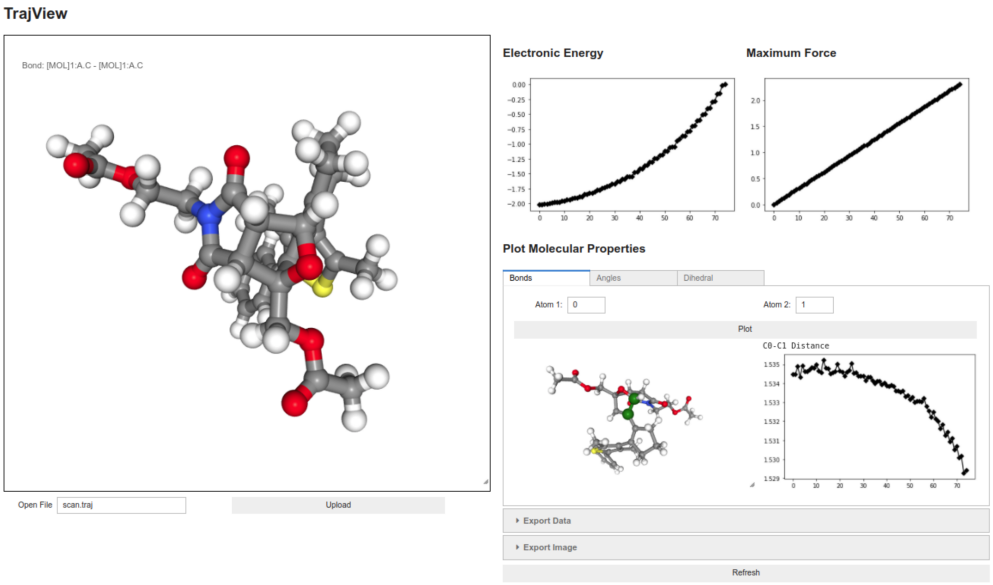
I developed a Python based module for pulling and pushing simulations that can work with the Atomic Simulation Environment (ASE) which is a Python framework. This can them be pathced with variety of quantum chemical software packages such as Gaussian, Q-Chem, DFTB+ among others. This is a significant contribution for the computational mechanochemistry community because only a single QM package has module for mechanochemical pulling. This paves the way for novel research by providing a readily available tool for mechanochemical simulations.



TrajView

Hokkaido University

In addition to algorithm development for chemical simulations, I also have experience in developing GUI using Python for chemistry applications. I developed TrajView which is a molecular trajectory viewer application which utilizes Voila, IPython, PyPlot, NumPy and ASE. This allows the user to view molecular trajectories. The application window also displays energies and forces during the trajectory. TrajView includes a molecular property plotting tool. This allows the use to plot bonds, angles, and dihedrals. Additionally, the plotted property is simultaneously visualized on the side. Data and image export is also possible.



CONFERENCE PRESENTATIONS

Total Presentations: 9 Poster (5 International , 4 Local) ; 1 Oral (Local)

Mechanical Pushing Induced Selective Cyclopropanation Reaction in Ag(111) Surface

Advanced School on Quantum Transport using Siesta

May 17 – 21 2021 San Sebastian, Spain (online)

Electronic Structure Understanding of the Mechanically Induced Selectivity in Acid Catalyzed Chitin Hydrolysis

9th Asia-Pacific Association of Theoretical and Computational Chemists

September 30- October 3, 2019 Sydney, Australia

Mechanochemical Selective Activation in Competing Chitin Hydrolysis Reactions

99th Spring Meeting of the Chemical Society of Japan 日本化学会第**99**春季年会

March 16-19, 2019 Kobe, Japan

Electronic Structure Origin of Mechanochemically Activated Chitin Depolymerization

4th National Symposium on Material Chemistry 合物化学研究推第**4**回国内シンポジウム

October 29-30, 2018 Kyushu, Japan

Theoretical Insights in Mechanochemical Selective Chitin Hydrolysis

Pre-conference of TOCAT8 and the 5th International Symposium of Institute for Catalysis)

August 3-4, 2018 Hokkaido, Japan

Theoretical Analysis of Mechanically Induced Selective Hydrolysis of Chitin

16th International Congress of Quantum Chemistry (16-ICQC)

June 18-23, 2018 Menton, France

Theoretical study for selective mechanochemical activation in chitin hydrolysis

Symposium on Nanomaterials for Environmental Purification and Energy Conversion

February 20-21, 2018 Hokkaido, Japan

Directional Dependence of Ea Changes in Mechanochemical Activation

Car-Parinello Molecular Dynamics Workshop 2017

October 18 - 20, 2017 Tsukuba, Japan

Structure-Based Pharmacophore Generation and Virtual Screening of Possible Inhibitors of Homology Modeled Plasmodium falciparum Signal Peptide Peptidase

Philippine Chemistry Congress

April 9 – 11, 2014 Camarines Sur, Philippines

RESEARCH PUBLICATIONS

Revisiting Activity Tuning using Lattice Strain: CO Decomposition in Terrace Ru(0001) and Stepped Ru(1015) Surfaces [Supplementary Journal Cover]

***D. P. De Chavez*, J. Hasegawa**

2022 | Journal of Physical Chemistry C

DOI: 10.1021/acs.jpcc.2c00902

OpenMechanochem : A Python module for mechanochemical simulations

***D. P. De Chavez*, J. Hasegawa**

2021 | SoftwareX

DOI:10.1016/j.softx.2021.100879 | https://pypi.org/project/OpenMechanochem/1.0.1/

On the Electronic Structure Origin of Mechanically Induced Selectivity in Acid Catalyzed Chitin Hydrolysis [Supplementary Journal Cover]

***D. P. De Chavez*, H. Kobayashi, A. Fukuoka, J. Hasegawa**

2020 | Journal of Physical Chemistry A

DOI:10.1021/acs.jpca.0c09030

Adsorption Mediated Tandem Acid Catalyzed Cellulose Hydrolysis by Ortho-substituted Benzoic Acids

***D. P. De Chavez*, M. Gao, H. Kobayashi, A. Fukuoka, J. Hasegawa**

2019 | Molecular Catalysis

DOI: 10.1016/j.mcat.2019.110459

Mechanical Pushing Induced Selective Cyclopropanation Reaction in Ag(111) Surface

***D. P. De Chavez*, J. Hasegawa**

2022 (In Preparation)

Extending Nudged Elastic Band to Mechanochemical Simulations: Minimum Energy Pathways in Modified Potential Energy Surfaces

***D. P. De Chavez*, J. Hasegawa**

2022 (In Preparation)