

Gwee Shu Hui Eunice

Email: eunice.gsh1990@gmail.com/eunice_gwee@icredd.hokudai.ac.jp

Experience

I am a highly motivated and skilled scientist that is interested in furthering my research in biomolecules, using both a computational and experimental approach. Currently, I am a Postdoctoral Fellow at Hokkaido University with A/Prof Hijikata, interested in modelling hormone flow in plant roots.

Publications

Pedroso, M. M., Larrabee, J. A., Ely, F., Gwee, S. E., Mitić, N., Ollis, D. L., Ollis & Schenk, G. (2016). CaII binding regulates and dominates the reactivity of a transition-metal-ion-dependent diesterase from *Mycobacterium tuberculosis*. *Chemistry-A European Journal*, 22(3), 999-1009.

Puntharod, R., Haller, K. J., Robertson, E. G., Gwee, E. S., Izgorodina, E. I., & Wood, B. R. (2017). An improved model for malaria pigment and β -hematin: Fe (OEP) picrate. *Journal of Raman Spectroscopy*, 48(9), 1148-1157.

Stevens, M. A., Hashim, F. H., Gwee, E. S., Izgorodina, E. I., Mulvey, R. E., & Blair, V. L. (2018). Contrasting Synergistic Heterobimetallic (Na-Mg) and Homometallic (Na or Mg) Bases in Metallation Reactions of Dialkylphenylphosphines and Dialkylanilines: Lateral versus Ring Selectivities. *Chemistry-A European Journal*, 24(58), 15669-15677.

Kochan, K., Peng, H., Gwee, E. S., Izgorodina, E., Haritos, V., & Wood, B. R. (2019). Raman spectroscopy as a tool for tracking cyclopropane fatty acids in genetically engineered *Saccharomyces cerevisiae*. *Analyst*, 144(3), 901-912.

Gwee, E. S., Seeger, Z. L., Appadoo, D. R., Wood, B. R., & Izgorodina, E. I. (2019). Influence of DFT Functionals and Solvation Models on the Prediction of Far-Infrared Spectra of Pt-Based Anticancer Drugs: Why Do Different Complexes Require Different Levels of Theory?. *ACS Omega*, 4(3), 5254-5269.

Education

Doctor of Philosophy Majoring in the Field of Chemistry	Monash University	2016 - 2021
Bachelor of Science (First Class Honours) Majoring in the Field of Chemistry	The University of Queensland, Australia	2015
Bachelor of Science Majoring in the Field of Chemistry	The University of Queensland, Australia	2011 - 2014

Work/Research Experience

- Nov 2018 **National Institute of Advanced Industrial Science and Technology,
Tsukuba, Tokyo, Japan**
- Worked with Dr Dmitri Fedorov, one of the developers of Fragment Molecular Orbital (FMO) method
 - The placement was to better understand the method and how to increase efficiency in studying larger systems
- Feb 2018 – June 2018 **School of Chemistry,
Monash University, Australia**
Lab Demonstration
- Lab demonstration for Year 3 Physical Chemistry Unit
 - Assisted the students in learning Unix commands and understand the basics of Computational Chemistry
 - Helping the students link the theoretical results back to Chemistry
- June 2015 – August 2015 **School of Chemistry and Molecular Bioscience,
The University of Queensland, Australia**
Research Assistant
- Taking a computational approach to study the active site and mechanism of the metallophosphoesterase, Rv0805.
 - To work on a paper for publication
- Feb 2015 – June 2015 **School of Chemistry and Molecular Biosciences,
The University of Queensland, Australia**
Lab Demonstration
- Lab demonstration for Year 1 Chemistry
 - Involved in lab safety, giving student directions when necessary and marking of lab report
- June 2014 – November 2014 **Women's College**
Math Tutor
- Prepare and aid the students in understanding the concepts of their Math courses (MATH1050, MATH1051, MATH1052)
 - Prepare the students for examinations

Skills and Abilities

Computer Software Knowledge

- ChemBioDraw Ultra
- Gaussian
- Pymol
- Cylview
- Mercury
- Avogadro
- Molden
- GAMESS

- Python
- R
- Unix
- PSI4
- Infrared Spectroscopy
- Raman Spectroscopy

Native Language (Spoken and Written)

- English
- Mandarin

Referees

The following persons may be contacted and/or are willing to send reference letters on my behalf:

Prof Ekaterina Pas (Monash Computational Chemistry Group)
School of Chemistry, Monash University
Email: katya.pass@monash.edu

Prof Bayden Wood (Biospectroscopy Group)
School of Chemistry, Monash University
Email: bayden.wood@monash.edu

Dr Karmen Condic-Jurkic (Open Force Field Initiative)
Project Manager at Open Force Field Initiative, New York
Email: karmen.condic-jurkic@choderalab.org

A/Prof Yuh Hijikata (Hokkaido University)
Email: hijikata@icredd.hokudai.ac.jp