



DEMONSTRATION SCHOOL,
UNIVERSITY OF PHAYAO



Assoc.Prof.Dr. Wijitra Jitonnorn

Research Interest

- Synthesis and kinetics of biodegradable polymer
- Theoretical studies on organometallic catalysis
- QM/MM study on enzymatic reactions
- Computer-aided drug design

Work

2012-present: Lecturer in Chemistry, Demonstration School University of Phayao and Physical Chemistry, School of Science, University of Phayao

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Education

2002-2006: B.Sc. (Industrial Chemistry)
Chiang Mai University

2007-2012: Ph.D. (Chemistry)
Chiang Mai University

Certificate

- Workshop Certificate (40 hours) awarded by the University of the Basque Country, Spain, 2017.
- Certificate for attending the 1st International Conference for Students in Science and Innovation awarded by the Institute for the Promotion of Teaching Science and Technology, 2020.
- Certificate for attending the 5th KVIS Invitational Science Fair awarded by Kamnoetvidya Science Academy, 2022.

Conference/Visiting Researcher

- 1) Visiting in the Brian J. Tighe 's group for training in "Practical techniques in Polymer Characterisation" at the Biomaterials research unit, Aston University, England, 2011.
- 2) Attending the 15th Asian Chemical Congress (15ACC), Singapore, 2013.
- 3) Attending the 4th Federation of Asian Polymer Societies-International Polymer Congress (4th FAPS-IPC), Kuala Lumpur, Malaysia, 2015.
- 4) Joining the Computational Chemistry Conference hosted by Donostia International Physics Center (DIPC) and Faculty of Chemistry at the University of the Basque Country (UPV/EHU), San Sebastian, Spain, 2017.
- 5) Attending the 7th International Conference on the Development of Biomedical Engineering at Vietnam National University, Ho Chi Minh City, Vietnam, 2018.
- 6) A short-term research scholar on "Computational modelling of catalysis focussing on transition metal assisted catalysis" at the Inorganic and Analytical Chemistry Department, Budapest University of Technology and Economics (BUTE), Budapest Hungary, 2019.
- 7) Attending CHARMM-GUI KIAS School workshop at, Korea Institute for Advanced Study (KIAS), Seoul, Korea, 2019.
- 8) A short-term research scholar on "Advanced materials and biomolecular science" at the Department of Chemistry and Biomedical Sciences, Linnaeus University, Sweden, 2022.
- 9) Attending the International Student Congress at Medical University of Graz, Austria, 2019-2025.

1. Meelua, W., Wanjai, T., Linnolahti, M., Jitonnorn, J., Origin of Comonomer Reactivity in Zirconocene-Mediated Polymerization of 2-Oxazoline and ϵ -Caprolactone: Insights from DFT, **Organometallics**, 2025, 44(16), 1764-1779. Scopus Q2
2. Protonation State of Active-Site Histidines, Reaction Mechanism and Stereoselectivity in β -Alanine Synthase: A Computational Study, **Journal Physical Chemistry B**, 2025, 129(23), 5664-5673. Scopus Q2
3. Meelua, W., Wanjai, T., Linnolahti, M., Jitonnorn, J., Ligand Structure Effects on the Stability of Cationic Zirconocene Dimethylaniline Complexes: Insights from Density Functional Theory, **ACS Omega**, 2025, 10(22), 23001-23010. Scopus Q1
4. Meelua, W., Wanjai, T., Jitonnorn, J., Exploring the effect of Zr/B ratio on the stability and reactivity of activated ϵ -caprolactone complexes: A DFT, QAIM and NCI study, **J. Mol. Graphics Model.**, 2025, 136, 108960. Scopus Q1
5. Meelua, W., Wanjai, T., Oláh, J., Linnolahti, M., Jitonnorn, J., Steric and Electronic Effects of Zirconocenealkyl-Borate Ion Pairs on Catalyst Activation: A Theoretical Study, **ACS Omega**, 2025, 10(1), 1082-1093. Scopus Q1
6. Meelua, W., Wanjai, T., Jitonnorn, J., Computational evaluation of zirconocene catalysts for ϵ -caprolactone cationic ring-opening polymerization, **Scientific Reports**, 2024, 14(1), 3952. Scopus Q1
7. Tue-ngeun, P., Rakitikul, W., Thinkumrob, N., ... Meelua, W., Jitonnorn, J., Binding interactions and in silico ADME prediction of isoconessimine derivatives as potent acetylcholinesterase inhibitors, **Journal of Molecular Graphics and Modelling**, 2024, 129, 108746. Scopus Q1
8. Jitonnorn, J., Meelua, W., Tue-nguen, P., et al, 3D-QSAR and molecular docking studies of peptide-hybrids as dengue virus NS2B/NS3 protease inhibitors, **Chemico Biological Interactions**, 2024, 396, 111040. Scopus Q1
9. Meelua, W., Linnolahti, M., Jitonnorn, J., Mechanism of cationic ring-opening polymerisation of ϵ -caprolactone using metallocene/borate catalytic systems: a DFT and NCI study on chain initiation, propagation and termination, **RSC Advances**, 2024, 14(17), 11715-11727. Scopus Q1
10. Meelua, W., Jitonnorn, J., DFT study of sucrose hydrolysis by a GH32 cell-wall invertase, a key enzyme in carbohydrate metabolism, **Molecular Simulation**, 2024, 50(4), 298-307. Scopus Q2
11. Meelua W., Thinkumrob N., Saparpakorn P., Pengthaisong S., Hannongbua S., Ketudat-Cairns J.R., Jitonnorn J., Structural basis for inhibition of a GH116 β -glucosidase and its missense mutants by GBA2 inhibitors: Crystallographic and quantum chemical study, **Chemico Biological Interactions**, 2023, 384, 110717. Scopus Q1
12. Meelua, W., Wanjai, T., Chokbunpiam, T., Jitonnorn, J., Mechanism of ring-opening polymerization of l-lactide by lanthanide aryloxide: A theoretical study on the effect of the aryloxide ligands on the process, **International Journal of Quantum Chemistry**, 2023, 123(16), e27134. Scopus Q2
13. Meelua, W., Wanjai, T., Thinkumrob, N., Friedman, R., Jitonnorn, J., Multiscale QM/MM Simulations Identify the Roles of Asp239 and 1-OH...Nucleophile in Transition State Stabilization in Arabidopsis thaliana Cell-Wall Invertase 1, **Journal of Chemical Information and Modeling**, 2023, 63(15), 4827-4838. Scopus Q1/Tier 1
14. Meelua, W., Wanjai, T., Thinkumrob, N., O. Julianna, J.R.Ketudat Cairns.. Ryde, S. Hannongbua, U., Jitonnorn, J., A computational study of the reaction mechanism and stereospecificity of dihydropyrimidinase, **Physical Chemistry Chemical Physics**, 2023, 25(12), 8767-8778. Scopus Q1
15. Meelua, W., Oláh, J., Jitonnorn, J., Role of water coordination at zinc binding site and its catalytic pathway of dizinc creatininase: insights from quantum cluster approach, **Journal of Computer Aided Molecular Design**, 2022, 36(4), 279-289. Scopus Q1
16. Limwanich, W., Meelua, W., Meepowpan, P., Punyodom, W., Kinetics and thermodynamics studies of the ring-opening polymerization of ϵ -caprolactone initiated by titanium(IV) alkoxides by isothermal differential scanning calorimetry, **Reaction Kinetics Mechanisms and Catalysis**, 2022, 135(2), 881-895. Scopus Q3
17. Meelua W., Wanjai T., Thinkumrob N., Oláh J., Mujika J.I., Ketudat-Cairns J.R., Hannongbua S., Jitonnorn J., Active site dynamics and catalytic mechanism in arabinan hydrolysis catalyzed by GH43 endo-arabinanase from QM/MM molecular dynamics simulation and potential energy surface, **Journal of Biomolecular Structure and Dynamics**, 2022, 40(16), 7439-7449. Scopus Q1
18. Jitonnorn, J., Meelua, W., DFT study of lactide ring-opening polymerizations by aluminium trialkoxides: Understanding the effects of monomer, alkoxide substituent, solvent and metal, **Chemical Physics Letters**, 2020, 750, 13748. Scopus Q1
19. Meelua, W., Keawkla, N., Oláh, J., Jitonnorn, J., DFT study of formation and properties of dinuclear zirconocene cations: Effects of ligand structure, solvent, and metal on the dimerization process, **Journal of Organometallic Chemistry**, 2020, 905, 121024. Scopus Q2
20. Jitonnorn, J., Meelua, W., Data on electronic structures for the study of ligand effects on the zirconocene-mediated trimethylene carbonate polymerization, **Data in Brief**, 2018, 20, 1867-1869. Scopus Q2

Publication

21. Jitonnom, J., Molloy, R., Punyodom, W., Meelua, W., The use of aluminum trialkoxide for synthesis of poly (ϵ -caprolactone) and poly (δ -valerolactone): A comparative study, **Songklanakarinn Journal of Science and Technology**, 2018, 40(4), 854-859. Scopus Q3
22. Jitonnom, J., Meelua, W., Cationic ring-opening polymerization of cyclic carbonates and lactones by group 4 metallocenes: A theoretical study on mechanism and ring-strain effects, **Journal of Theoretical and Computational Chemistry**, 2017, 16(1), 1750003. Scopus Q3
23. Jitonnom, J., Meelua, W., Effect of ligand structure in the trimethylene carbonate polymerization by cationic zirconocene catalysts: A "naked model" DFT study, **Journal of Organometallic Chemistry**, 2017, 841, 48-56. Scopus Q2
24. Jitonnom, J., Molloy, R., Punyodom, W., Meelua, W., Theoretical studies on aluminum trialkoxide-initiated lactone ring-opening polymerizations: Roles of alkoxide substituent and monomer ring structure, **Computational and Theoretical Chemistry**, 2016, 1097, 25-32. Scopus Q2
25. Jitonnom, J., Meelua, W., Effects of silicon-bridge and π -ligands on the electronic structures and related properties of dimethyl zirconocene polymerization catalysts: A comparative theoretical study, **Chiang Mai Journal of Science**, 2014, 41(5-2), 1220-1229. Scopus Q3
26. Meelua, W., Bua-Own, V., Molloy, R., Punyodom, W., Comparison of metal alkoxide initiators in the ring-opening polymerization of caprolactone, **Advanced Materials Research**, 2012, 506, 142-145. Scopus
27. Meelua, W., Molloy, R., Meepowpan, P., Punyodom, W., Isoconversional kinetic analysis of ring-opening polymerization of ϵ -caprolactone: Steric influence of titanium(IV) alkoxides as initiators, **Journal of Polymer Research**, 2012, 19(2), 9799. Scopus Q2