Asst. Prof. Dr. Wijitra Meelua

Education

2002-2006	B.Sc. (Industrial Chemistry) Chiang Mai University
2007-2012	Ph.D. (Chemistry) Chiang Mai University

Work

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

Research Interest

- Polymerization characterization and kinetics
- Computational studies on organometallic and enzyme catalysis

Publications

1. **Meelua, W**., Oláh, J., and Jitonnom, 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**) *Just accepted*, (Indexed in WoS IF 2020 = 3.686)
2. Limwanich, W., **Meelua, W.,** Meepowpan, P. et al. Kinetics and thermodynamics studies of the ring-opening polymerization of ε-caprolactone initiated by titanium(IV) alkoxides by isothermal differential scanning calorimetry. Reac Kinet Mech Cat (**2022**). https://doi.org/10.1007/s11144-022-02184-z, (Indexed in WoS IF 2020 = 1.7)
3. **Meelua, W**., Wanjai, T., Thinkumrob, N., Oláh, J., Mujika, J.I., Ketudat-Cairns, J.R., Hannongbua, S., and Jitonnom, 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, (**2021**) DOI: 10.1080/07391102.2021.1898469, (Indexed in WoS IF 2019 = 3.310)

4. Jitonnom J., **Meelua W.** J. DFT Study of Lactide Ring-Opening Polymerizations by Aluminium Trialkoxides: Understanding the Effects of Monomer, Alkoxide Substituent, Solvent and Metal. Chem. Phys. Lett., **2020**, 750, 137482 (Indexed in WoS IF 2020 = 2.328)
5. **Meelua W.,** Keawkla N., Oláh J., Jitonnom, J. DFT study of formation and properties of dinuclear zirconocence cations: Effects of ligand structure, solvent, and metal on the dimerization process. J. Organometal. Chem., **2020**, 905, 121024. (Indexed in WoS IF 2020 = 2.369)
6. 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. Songklanakarin J. Sci. Tech., **2018**, 40(4), 854-859. (Indexed in Scopus)
7. Jitonnom J., **Meelua W**. Data on electronic structures for the study of ligand effects on the zirconocene-mediated trimethylene carbonate polymerization. Data Brief., **2018**, 20, 1867-1869. (Indexed in Scopus)
8. Jitonnom J., **Meelua W.** Effect of ligand structure in the trimethylene carbonate polymerization by cationic zirconocene catalysts: A "naked model" DFT study. J. Organometal. Chem., **2017**, 841, 48-56. (Indexed in WoS IF = 2.066)
9. 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. J. Theor. Comp. Chem., **2017**, 16(1), 1750003. (Indexed in WoS IF = 0.60)
10. Jitonnom J., Molloy R., Punyodom W., **Meelua W.** Theoretical studies on aluminumtrialkoxide-initiated lactone ring-opening polymerizations: Roles of alkoxide substituentand monomer ring structure. Comput. Theor. Chem. **2016**, 1097, 25-32. (Indexed in WoS IF = 1.344)
11. **Meelua W.**, Jitonnom J. Effects of Silicon-Bridge and pi-Ligands on the Electronic Structures and Related Properties of Dimethyl Zirconocene Polymerization Catalysts: A Comparative Theoretical Study, Chiang Mai J. Sci., **2014**, 41: 1220–1229. (Indexed in WoS IF = 0.342)
12. **Meelua W.**, Molloy R., Meepowpan P., Punyodom W. Isoconversional kinetic analysis of ring-opening polymerization of Ɛ-caprolactone: Steric influence of titanium(IV) alkoxides as initiators, J. Polym. Res., **2012**, 19: 1-11. (Indexed in WoS IF = 1.53)

13. **Meelua W.**, Bua-Own V., Molloy R., Punyodom W. Comparison of metal alkoxide initiators in the ring-opening polymerization of caprolactone, Adv. Mat. Res., **2012**, 506: 142-145. (Indexed in WoS IF = 0.87)