



**Asst. Prof. Dr. Nawee Kungwan**

**Office address:**

Department of Chemistry, Faculty of Science,  
Chiang Mai University, Chiang Mai, Thailand 50200  
Tel: +66-53-943336 Ext. 126 or cell phone +66-84-8283641  
Fax: +66-53-892277  
Email: naweekung@gmail.com, nawee.kungwan@cmu.ac.th  
Website: www.ccl-cmu.com

**Profession:**

2007-2014                      Lecturer, Chiang Mai University  
2014-present                 Assistant Professor, Chiang Mai University

**FIELDS OF SPECIALIZATION:**

Computational Chemistry (dye-sensitized solar cells, light emitting materials, catalyst in ring-opening polymerization, catalytic materials for hazardous gas adsorption, excited-state proton transfer and molecular design for fluorescent probes)

**Educational background**

2000    BSc (Chemistry) Department of Chemistry, Khon Kaen University, Khon Kaen, Thailand  
2007    PhD (Chemistry) Chemistry Department, University of Utah, Salt Lake City, Utah, USA  
2009    Postdoc researcher, Institute for Theoretical Chemistry, University of Vienna, Vienna, Austria

**Training and short visit:**

2013 (April-May, 2 months) Visiting researcher, Quantum Physical Chemistry Group, Yokohama City University, Yokohama, Japan.  
2013 (June-August, 2 months) Visiting researcher, Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany.  
2014 (January-February, 2 months) Visiting researcher, Quantum Physical Chemistry Group, Yokohama City University, Yokohama, Japan.

2015 (March-April, 2 months) Visiting researcher supported by DAAD through German-Thai Mobility Grant, Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany.

2015 (August, 1 month) Visiting researcher supported by The Hitachi Global Foundation, Department of Chemistry, Nagoya University, Japan.

2016 (January, 3 weeks) Visiting researcher supported by Travel grant from Kyoto University, Quantum Physical Chemistry Group, Yokohama City University, Yokohama, Japan.

2016 (May-July, 3 months) Visiting researcher, Theoretical and Computational Chemistry Group, Queen Mary University of London, London, UK.

2016 (August, 3 weeks) Visiting researcher supported by SAKURA Exchange Program in Science, University, Quantum Physical Chemistry Group, Yokohama City University, Yokohama, Japan.

2017 (July, 3 weeks) Visiting researcher supported by SAKURA Exchange Program in Science, University, Quantum Physical Chemistry Group, Yokohama City University, Yokohama, Japan.

2018 (June-July, 6 weeks) Visiting researcher supported by Institute de Chimie Radicalaire, Aix-Marseille University, Marseille, France.

2018 (July-August, 3 weeks) Visiting researcher supported by SAKURA Exchange Program in Science, University, Quantum Physical Chemistry Group, Yokohama City University, Yokohama, Japan.

**Awards:**

- The highest impact factor publication awarded by Faculty of Science, Chiang Mai University (Chemical Science IF=9.211(2015))
- The recipient of Golden Elephant Award for Young Researcher from Chiang Mai University in 2016
- Middle Career Researcher Award, given by Faculty of Science, Chiang Mai University, Year 2017

**Project Funds:**

- Thailand Research Fund (TRF) Research Career Development Grant. 2018-2021
- TRF Research Career Development Grant, 2015-2018
- TRF Research Grant for New Scholar, 2013-2015
- TRF Research Grant for New Scholar, 2011-2013

**Bibliographic Indicators:** Peer-reviewed papers: 124 (2005-2019)

Citations: 930 – H-index: 14 (Scopus, 30 January 2019)

ORCID: [orcid.org/0000-0002-2960-6853](https://orcid.org/0000-0002-2960-6853); Scopus Author ID: 16417107900

Full publication list: [www.scopus.com/authid/detail.uri?authorId=16417107900](http://www.scopus.com/authid/detail.uri?authorId=16417107900)

### Selected Publications:

1. Salaeh, R.; Prommin, C.; Chansen, W.; Kerdpol, K.; Daengngern, R.; Kungwan, N., The Effect of Protic Solvents on the Excited State Proton Transfer of 3-Hydroxyflavone: A Td-Dft Static and Molecular Dynamics Study. *J. Mol. Liq.* 2018, 252, 428-438.
2. Saelee, T.; Namuangruk, S.; Kungwan, N.; Junkaew, A., Theoretical Insight into Catalytic Propane Dehydrogenation on Ni(111). *J. Phys. Chem. C* 2018, 122, 14678-14690.
3. Li, Y.; Sun, C.; Song, P.; Ma, F.; Kungwan, N.; Sun, M., Physical Insight on Mechanism of Photoinduced Charge Transfer in Multipolar Photoactive Molecules. *Scientific Reports* 2018, 8.
4. Daengngern, R.; Camacho, C.; Kungwan, N.; Irle, S., Theoretical Prediction and Analysis of the Uv/Visible Absorption and Emission Spectra of Chiral Carbon Nanorings. *J. Phys. Chem. A* 2018, 122, 7284-7292.
5. Yuan, F.; Li, J.; Namuangruk, S.; Kungwan, N.; Guo, J.; Wang, C., Microporous, Self-Segregated, Graphenel Polymer Nanosheets Prepared by Dehydrogenative Condensation of Aza-Pahs Building Blocks in the Solid State. *Chemistry of Materials* 2017, 29, 3971-3979.
6. Suda, M.; Takashina, N.; Namuangruk, S.; Kungwan, N.; Sakurai, H.; Yamamoto, H. M., N-Type Superconductivity in an Organic Mott Insulator Induced by Light-Driven Electron-Doping. *Advanced Materials* 2017, 29.
7. Sattayanon, C.; Namuangruk, S.; Kungwan, N.; Kunaseth, M., Reaction and Free-Energy Pathways of Hydrogen Activation on Partially Promoted Metal Edge of Comos and Nimos: A Dft and Thermodynamics Study. *Fuel Process. Technol.* 2017, 166, 217-227.
8. Prommin, C.; Kanlayakan, N.; Chansen, W.; Salaeh, R.; Kerdpol, K.; Daengngern, R.; Kungwan, N., Theoretical Insights on Solvent Control of Intramolecular and Intermolecular Proton Transfer of 2-(2'-Hydroxyphenyl)Benzimidazole. *J. Phys. Chem. A* 2017, 121, 5773-5784.
9. Manojai, N.; Daengngern, R.; Kerdpol, K.; Ngaojampa, C.; Kungwan, N., Heteroatom Effect on Photophysical Properties of 2-(2'-Hydroxyphenyl)Benzimidazole and Its Derivatives as Fluorescent Dyes: A Td-Dft Study. *J. Lumin.* 2017, 188, 275-282.
10. Kungwan, N.; Ngaojampa, C.; Ogata, Y.; Kawatsu, T.; Oba, Y.; Kawashima, Y.; Tachikawa, M., Solvent Dependence of Double Proton Transfer in the Formic Acid-Formamidine Complex: Path Integral Molecular Dynamics Investigation. *J. Phys. Chem. A* 2017, 121, 7324-7334.
11. Kanlayakan, N.; Kerdpol, K.; Prommin, C.; Salaeh, R.; Chansen, W.; Sattayanon, C.; Kungwan, N., Effects of Different Proton Donor and Acceptor Groups on Excited-State Intramolecular Proton Transfers of Amino-Type and Hydroxy-Type Hydrogen-Bonding Molecules: Theoretical Insights. *New J. Chem.* 2017, 41, 8761-8771.
12. Chansen, W.; Salaeh, R.; Prommin, C.; Kerdpol, K.; Daengngern, R.; Kungwan, N., Theoretical Study on Influence of Geometry Controlling over the Excited-State Intramolecular Proton Transfer of 10-Hydroxybenzo[H]Quinoline and Its Derivatives. *Comput. Theor. Chem.* 2017, 1113, 42-51.
13. Tan, J.; Namuangruk, S.; Kong, W.; Kungwan, N.; Guo, J.; Wang, C., Manipulation of Amorphous-to-Crystalline Transformation: Towards the Construction of Covalent Organic Framework Hybrid Microspheres with Nir Photothermal Conversion Ability. *Angewandte Chemie - International Edition* 2016, 55, 13979-13984.
14. Meeprasert, J.; Junkaew, A.; Kungwan, N.; Jansang, B.; Namuangruk, S., A Cr-Phthalocyanine Monolayer as a Potential Catalyst for No Reduction Investigated by Dft Calculations. *RSC Advances* 2016, 6, 20500-20506.

15. Sattayanon, C.; Sontising, W.; Limwanich, W.; Meepowpan, P.; Punyodom, W.; Kungwan, N., Effects of Alkoxide Alteration on the Ring-Opening Polymerization of  $\epsilon$ -Caprolactone Initiated by N-Bu<sub>3</sub>Sn: A DFT Study. *Structural Chemistry* 2015, 26, 695-703.
16. Kerdpol, K.; Daengngern, R.; Kungwan, N., Excited-State Proton-Transfer Reactions of 7-Azaindole with Water, Ammonia and Mixed Water-Ammonia: Microsolvated Dynamics Simulation. *Molecular Simulation* 2015, 41, 1177-1186.
17. Daengngern, R.; Kungwan, N., Electronic and Photophysical Properties of 2-(2'-Hydroxyphenyl)Benzoxazole and Its Derivatives Enhancing in the Excited-State Intramolecular Proton Transfer Processes: A Td-Dft Study on Substitution Effect. *Journal of Luminescence* 2015, 167, 132-139.
18. Crespo-Otero, R.; Kungwan, N.; Barbatti, M., Stepwise Double Excited-State Proton Transfer Is Not Possible in 7-Azaindole Dimer. *Chemical Science* 2015, 6, 5762-5767.
19. Sattayanon, C.; Sontising, W.; Jitonnorn, J.; Meepowpan, P.; Punyodom, W.; Kungwan, N., Theoretical Study on the Mechanism and Kinetics of Ring-Opening Polymerization of Cyclic Esters Initiated by Tin(II) N-Butoxide. *Computational and Theoretical Chemistry* 2014, 1044, 29-35.
20. Kungwan, N.; Ogata, Y.; Hannongbua, S.; Tachikawa, M., Nuclear Quantum Effect and Temperature Dependency on the Hydrogen-Bonded Structure of 7-Azaindole Dimer. *Theoretical Chemistry Accounts* 2014, 133, 1-10.
21. Kungwan, N.; Khongpracha, P.; Namuangruk, S.; Meeprasert, J.; Chitpakdee, C.; Jungsuttiwong, S.; Promarak, V., Theoretical Study of Linker-Type Effect in Carbazole–Carbazole-Based Dyes on Performances of Dye-Sensitized Solar Cells. *Theoretical Chemistry Accounts* 2014, 133, 1-14.
22. Kungwan, N.; Kerdpol, K.; Daengngern, R.; Hannongbua, S.; Barbatti, M., Effects of the Second Hydration Shell on Excited-State Multiple Proton Transfer: Dynamics Simulations of 7-Azaindole: (H<sub>2</sub>O)<sub>1-5</sub> Clusters in the Gas Phase. *Theoretical Chemistry Accounts* 2014, 133, 1-11.
23. Daengngern, R.; Kungwan, N., Dynamics Simulations of Photoinduced Proton Transfer Reactions of 2-(2'-Hydroxyphenyl)Benzoxazole in the Gas Phase and Its Hydrated Clusters. *Chemical Physics Letters* 2014, 609, 147-154.