Thantip Roongcharoen

Position: Early-stage researcher / Ph.D. candidate

Affiliation I: Via G. Moruzzi, 1 - 56124 Pisa, Italy
Institute of Chemistry of Organometallic Compounds,
National Research Council of Italy (CNR-ICCOM)

Affiliation II: National Nanotechnology Center (NANOTEC), National Science and Technology Development Agency (NSTDA), Thailand

E-mail: [redacted]

Nationality: Thai

Education and Experience:

June 2013 – May 2017	B.Sc. (Chemistry)	Chiang Mai University, Chiang Mai, Thailand
August 2017 – May 2019	M.Sc. (Chemistry)	Chiang Mai University, Chiang Mai, Thailand
June 2019 – July 2020	Research Assistant	NANOTEC, Thailand
August 2020 – Present	Ph.D. candidate (Chemistry)	University of Pisa, Pisa, Italy

Scholarship and Funding Support:

2014–2016	Thai Bridgestone Scholarships
2016	Young Scientist and Technologist Programme, NANOTEC
2017–2019	Thailand Graduate Institute of Science and Technology (TGIST), NANOTEC
2020–present	Bimetallic catalyst knowledge-based development for energy applications (BIKE), European Union's Horizon 2020 Research and Innovation programme under the Marie Skłodowska-Curie Action

Research Interests:

- Modelling Hydrogen Production via Aqueous Phase and Steam Reforming Catalysis (Ph.D. research)
- Design and Development of Efficient Catalysts for Energy Conversions

Publications:

1. **T. Roongcharoen**, X. Yang, S. Han, L. Sementa, L. Vegge, H.A. Hansen, A. Fortunelli, Oxidation and De-Alloying of PtMn particle models: a computational investigation, *Faraday Discuss., 2022, Advance Article*, doi: 10.1039/D2FD00107A.

2. **T. Roongcharoen,** P. Mano, T. Jitwatanasirikul, P. Sikam, T. Butburee, K. Takahashi, S. Namuangruk, 'Theoretical insight on why N-vacancy promotes the selective CO_2 reduction to Ethanol on NiMn doped Graphitic Carbon Nitride Sheets**',** *Applied Surface Science*, 2022, 595, 153527, doi: 10.1016/j.apsusc.2022.153527.

3. **T. Roongcharoen**, S. Impeng, T. Rungrotmongkol, T. Jitwatanasirikul, S. Jungsuttiwong, S. Namuangruk, 'Intrinsic property and catalytic performance of single and double metal atoms incorporated g-C_3N_4 for O_2 activation: A DFT insight', *Applied Surface Science*, 2021 148671, doi: 10.1016/j.apsusc.2020.148671.

4. **T. Roongcharoen**, S. Impeng, N**.** Kungwan, S. Namuangruk, 'Revealing the effect of N-content in Fe doped graphene on its catalytic performance for direct oxidation of methane to methanol', *Applied Surface Science*, 2020, 527, 146833, doi: 10.1016/j.apsusc.2020.146833.

5. **T. Roongcharoen**, N. Kungwan, R. Daengngern, C. Sattayanon, S. Namuangruk, 'Nitric oxide oxidation on warped nanographene ($C_{80}H_{30}$): a DFT study', *Theoretical Chemistry Accounts*, 2019, 1, 18, doi: 10.1007/s00214-018-2407-9.

6. F. Bossola, **T. Roongcharoen**, M. Coduri, C. Evangelisti, F. Somodi, L. Sementa, A. Fortunelli, V. Dal Santo, 'Discovering indium as hydrogen production booster for a Cu/SiO_2 catalyst in steam reforming of methanol', *Applied Catalysis B: Environmental*, 297 (2021) 120398, doi: 10.1016/j.apcatb.2021.120398.

7. S. Hadsadee, **T. Roongcharoen,** K. Takahashi, S. Namuangruk, Enhanced Electrocatalytic C_{O2} Reduction Reactivity by S and N Doping to Fe-Embedded Graphene, *ChemPlusChem*, 2023, e202300306, DOI: 10.1002/cplu.202300306

8. T. Jitwatanasirikul, **T. Roongcharoen**, P. Sikam, K. Takahashi, S. Namuangruk, 'The screening of homo- and hetero-dual atoms anchored graphdiyne for boosting the electrochemical CO_2 reduction', *Adv. Mater. Interfaces*, 10, 2201904, 2023, doi: https://doi.org/10.1002/admi.202201904

9. P. Sikam, T. Jitwatanasirikul, **T. Roongcharoen**, N. Yodsin, J. Meeprasert, K. Takahashi, S. Namuangruk, 'Understanding the interaction between transition metal doping and ligand atoms of ZnS and ZnO monolayers to promote the CO_2 reduction reaction', *Phys. Chem. Chem. Phys.*, 2022, 24, 12909-12921, dol: 10.1039/D2CP00878E

10. P. Sikam, K. Takahashi, **T. Roongcharoen**, T. Jitwatanasirikul, C. Chitpakdee, K. Faungnawakij, S. Namuangruk, 'Effect of 3d-transition metals doped in ZnO monolayers on the CO_2 electrochemical reduction to valuable products: first principles study', *Applied Surface Science*, 550 (2021) 149380, doi: 10.1016/j.apsusc.2021.149380.

11. T. Jitwatanasirikul, **T. Roongcharoen,** C. Chitpakdee, S. Jungsuttiwong, P. Poldorm, K. Takahashi, S. Namuangruk, 'Co-embedded sulfur vacant MoS_2 monolayer as a promising catalyst for formaldehyde oxidation: a theoretical evaluation', *New Journal of Chemistry*, 2021, 45, 17407-17417, doi: 10.1039/D1NJ02869C.

12. S. Impeng, **T. Roongcharoen**, P. Maitarad, H. Wu, C. Chitpakdee, V. Promarak, L. Shi, S. Namuangruk, 'High selective catalyst for ethylene epoxidation to ethylene oxide: A DFT investigation', *Applied Surface Science*, 2020, 513, 145799, doi**:** 10**.**1016/j**.**apsusc**.**2020**.**145799**.**

13. A**.** Watwiangkham, **T. Roongcharoen**, N**.** Kungwan, 'Effect of nitrogen substitution and π-conjugation on photophysical properties and excited state intramolecular proton transfer reactions of methyl salicylate derivatives: Theoretical investigation', *J. Photochem. Photobiol. A***:** *Chem*, 2020, 289, 112267, doi**:** 10**.**1016/j**.**jphotochem**.**2019**.**112267**.**

14. P. Praikaew, **T. Roongcharoen**, A. Charoenpanich, N. Kungwan, N. Wanichacheva, 'Near-IR aza-BODIPY-based probe for the selective simultaneous detection of Cu^{2+} in aqueous buffer solutions and its application in biological samples', *J. Photochem. Photobiol. A: Chem*, 2020, 400, 112641, doi**:** 10.1016/j.jphotochem.2020.112641.

15. T. Ungpittagul, T. Jaenjai, **T. Roongcharoen**, S. Namuangruk, K. Phomphrai, 'Unprecedented Double Insertion of Cyclohexene Oxide in Ring-Opening Copolymerization with Cyclic Anhydrides Catalyzed by a Tin(II) Alkoxide Complex', *Macromolecules*, 53 (2020) 9869-9877, doi: 10.1021/acs.macromol.0c01738.

16. H. T. Huynh, H. T. Phan, P. J. Hsu, J. L. Chen, H. S. Nguan, S. T. Tsai, **T. Roongcharoen**, C.Y. Liew, C. K. Ni, J. L. Kuo, 'Collision-induced dissociation of sodiated glucose, galactose, and mannose, and the identification of anomeric configurations', *Phys. Chem. Chem. Phys*., 2018, 20, 19614, doi: 10.1039/C8CP03753A.

Proceeding:

T. Roongcharoen, N. Kungwan, S. Namuangruk, 'A first principle study of gas adsorption on Fe-doped nitrogen-coordinated graphene', The Pure and Applied Chemistry International Conference 2019 (PACCON2019), 2019, PH7-PH12.

Supervisors and Advisor:

Dr. Alessandro Fortunelli (Supervisor)

CNR-ICCOM, Consiglio Nazionale delle Ricerche, Via G. Moruzzi 1, 56124, Pisa, Italy

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Dr. Luca Sementa (Co-Supervisor)

CNR- IPCF, Istituto per i Processi Chimico-Fisici, Via G. Moruzzi 1, 56124, Pisa, Italy

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Dr. Supawadee Namuangruk (Advisor)

National Nanotechnology Center **(**NANOTEC), Thailand

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Scientific Award

Poster Prize Award from *Catalysis Science & Technology* and *Faraday Discussion*s at the Cluster Meeting 2023, Prague, Czech Republic, 18th -23rd June 2023

Exchanges and Internships:

1. 1 June – 31 July 2017: Molecular Science and Technology research experience for Undergraduates Summer 2017 in International Graduate 2017 International Internship Program at Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan.
2. 30 July – 9 August 2018: Sakura Exchange Program in Science at Yokohama City University, Yokohama, Japan.
3. 22 November 2018 – 15 January 2019: International Internship Program **(**IAMS-IIP**)** at Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan**.**
4. 1 November 2021 – 15 December 2021: A Ph.D. guest at Atomic Scale Materials Modelling, Department of Energy Conversion and Storage, Technical University of Denmark (DTU), Denmark.
5. 16 November 2022 – 17 December 2022: A Ph.D. guest at Atomic Scale Materials Modelling, Department of Energy Conversion and Storage, Technical University of Denmark (DTU), Denmark.

Conference and workshop attendance:

1. Participant: Modern concepts and spectroscopic methods in materials science and catalysis lectures on 6th April – 27th July 2021 organized by KIT
2. Presenter: Project presentation seminars for Ph.D student on 19th -25th March 2021 organized by the Doctoral School in Chemistry and Material Science (DSCM), Department of Chemistry and Industrial of the University of Pisa
3. Participant: Theoretical Approaches to NanoAlloy Catalysis workshop on 16th -19th March 2021 organized by DTU
4. Poster Presenter: Cluster Meeting 2021 on 18th -23rd July 2021 at J. Heyrovský Institute, Prague, Czech Republic

Computer Skills:

Softwares: DMol^3, Gaussian, LAMMPS**,** VASP, Quantum Espresso

Language: Python

Tools: X-Crysden, VESTA, GaussView, MATERIAL STUDIO, ASE, Bash/Shell script

Platforms: Windows, Linux