

Li, Yi-Pei (李奕霏)

Assistant Professor

B.S. in Chemical Engineering
National Taiwan University, 2009

Ph.D. in Chemical Engineering
University of California at Berkeley, 2016

Research and Professional Interests

Reaction Engineering
Computational Chemistry
Machine Learning

Journal Papers

1. Yang, C.-I.; Li, Y.-P. , Explainable Uncertainty Quantifications for Deep Learning-Based Molecular Property Prediction, *Journal of Cheminformatics* , 15(1)13-2023
2. Matsagar, B. M.; Li, T.-H.; Van Chi, N.; Hossain, Md. S. A.; Ahamad, T.; Li, Y.-P.; Wu, K. C.-W, Furfural Hydrogenation into Tetrahydrofurfuryl Alcohol under Ambient Conditions: Role of Ni-Supported Catalysts and Hydrogen Source, *Industrial Crops and Products* , 195, 2023
3. Li, S.-C.; Lin, Y.-C.; Li, Y.-P. , Comparative Analysis of Uncoupled Mode Approximations for Molecular Thermochemistry and Kinetics, *Journal of Chemical Theory and Computation*, 18(11), 2022
4. Chen, L.-Y.; Hsu, T.-W.; Hsiung, T.-C.; Li, Y.-P. , Deep Learning-Based Increment Theory for Formation Enthalpy Predictions, *The Journal of Physical Chemistry A*, 126(41), 2022
5. Gong, Z.-J.; Narayana, Y. S. L. V.; Lin, Y.-C.; Huang, W.-H.; Su, W.-N.; Li, Y.-P.; Higuchi, M.; Yu, W.-Y. , Rational Synthesis of Ruthenium-Based Metallo-Supramolecular Polymers as Heterogeneous Catalysts for Catalytic Transfer Hydrogenation of Carbonyl Compounds, *Applied Catalysis B: Environmental* , 312, 2022
6. X. Li; T.-H. Li; W. Zhou; Y.-P. Li; P. H.-L. Sit; Z. Wu; O. J. Curnow; K. C.-W. Wu; J. Choi; A. C. K. Yip , Unveiling the Elusive Role of Tetraethyl Orthosilicate Hydrolysis in Ionic-Liquid-Templated Zeolite Synthesis, *Materials Today Chemistry* , 23, 2022
7. W. H. Ho; S.-C. Li; Y.-C. Wang; T.-E. Chang; Y.-T. Chiang; Y.-P. Li; C.-W. Kung, Proton-Conductive Cerium-Based Metal–Organic Frameworks, *ACS Applied Materials & Interfaces*, 13(46), 2021
8. S.-C. Li; Y.-C. Lin; Y.-P. Li , Understanding the Catalytic Activity of Microporous and Mesoporous Zeolites in Cracking by Experiments and Simulations, *Catalysts* , 11(9), 2021
9. Epifanovsky, E.; Gilbert, A. T. B.; Feng, X.; Lee, J.; Mao, Y.; Mardirossian, N.; Pokhilko, P.; White, A. F.; Coons, M. P.; Dempwolff, A. L.; Gan, Z.; Hait, D.; Horn, P. R.; Jacobson, L. D.; Kaliman, I.; Kussmann, J.; Lange, A. W.; Lao, K. U.; Levine, D. S.; Liu, J.; McKenzie, S. C.; Morrison, A. F.; Nanda, K. D.; Plasser, F.; Rehn, D. R.; Vidal, M. L.; You, Z.-Q.; Zhu, Y.; Alam, B.; Albrecht, B. J.; Aldossary, A.; Alguire, E.; Andersen, J. H.; Athavale, V.; Barton, D.; Begam, K.; Behn, A.; Bellonzi, N.; Bernard, Y. A.; Berquist, E. J.; Burton, H. G. A.; Carreras, A.; Carter-Fenk, K.; Chakraborty, R.; Chien, A. D.; Closser, K. D.; Cofer-Shabica, V.; Dasgupta, S.; de Wergifosse, M.; Deng, J.; Diedenhofen, M.; Do, H.; Ehlert, S.; Fang, P.-T.; Fatehi, S.; Feng, Q.; Friedhoff, T.; Gayvert, J.; Ge, Q.; Gidofalvi, G.; Goldey, M.; Gomes, J.; González-Espinoza, C. E.; Gulania, S.; Gunina, A. O.; Hanson-Heine, M. W. D.; Harbach, P. H. P.; Hauser, A.; Herbst, M. F.; Hernández Vera,

- M.; Hodecker, M.; Holden, Z. C.; Houck, S.; Huang, X.; Hui, K.; Huynh, B. C.; Ivanov, M.; Jász, Á.; Ji, H.; Jiang, H.; Kaduk, B.; Kähler, S.; Khistyayev, K.; Kim, J.; Kis, G.; Klunzinger, P.; Koczor-Benda, Z.; Koh, J. H.; Kosenkov, D.; Koulias, L.; Kowalczyk, T.; Krauter, C. M.; Kue, K.; Kunitsa, A.; Kus, T.; Ladjánszki, I.; Landau, A.; Lawler, K. V.; Lefrancois, D.; Lehtola, S.; Li, R. R.; Li, Y.-P.; Liang, J.; Liebenthal, M.; Lin, H.-H.; Lin, Y.-S.; Liu, F.; Liu, K.-Y.; Loipersberger, M.; Luenser, A.; Manjanath, A.; Manohar, P.; Mansoor, E.; Manzer, S. F.; Mao, S.-P.; Marenich, A. V.; Markovich, T.; Mason, S.; Maurer, S. A.; McLaughlin, P. F.; Menger, M. F. S. J.; Mewes, J.-M.; Mewes, S. A.; Morgante, P.; Mullinax, J. W.; Oosterbaan, K. J.; Paran, G.; Paul, A. C.; Paul, S. K.; Pavošević, F.; Pei, Z.; Prager, S.; Proynov, E. I.; Rák, Á.; Ramos-Cordoba, E.; Rana, B.; Rask, A. E.; Rettig, A.; Richard, R. M.; Rob, F.; Rossomme, E.; Scheele, T.; Scheurer, M.; Schneider, M.; Sergueev, N.; Sharada, S. M.; Skomorowski, W.; Small, D. W.; Stein, C. J.; Su, Y.-C.; Sundstrom, E. J.; Tao, Z.; Thirman, J.; Tornai, G. J.; Tsuchimochi, T.; Tubman, N. M.; Veccham, S. P.; Vydrov, O.; Wenzel, J.; Witte, J.; Yamada, A.; Yao, K.; Yeganeh, S.; Yost, S. R.; Zech, A.; Zhang, I. Y.; Zhang, X.; Zhang, Y.; Zuev, D.; Aspuru-Guzik, A.; Bell, A. T.; Besley, N. A.; Bravaya, K. B.; Brooks, B. R.; Casanova, D.; Chai, J.-D.; Coriani, S.; Cramer, C. J.; Cserey, G.; DePrince, A. E.; DiStasio, R. A.; Dreuw, A.; Dunietz, B. D.; Furlani, T. R.; Goddard, W. A.; Hammes-Schiffer, S.; Head-Gordon, T.; Hehre, W. J.; Hsu, C.-P.; Jagau, T.-C.; Jung, Y.; Klamt, A.; Kong, J.; Lambrecht, D. S.; Liang, W.; Mayhall, N. J.; McCurdy, C. W.; Neaton, J. B.; Ochsenfeld, C.; Parkhill, J. A.; Peverati, R.; Rassolov, V. A.; Shao, Y.; Slipchenko, L. V.; Stauch, T.; Steele, R. P.; Subotnik, J. E.; Thom, A. J. W.; Tkatchenko, A.; Truhlar, D. G.; Van Voorhis, T.; Wesolowski, T. A.; Whaley, K. B.; Woodcock, H. L.; Zimmerman, P. M.; Faraji, S.; Gill, P. M. W.; Head-Gordon, M.; Herbert, J. M.; Krylov, A. I., Software for the Frontiers of Quantum Chemistry: An Overview of Developments in the Q-Chem 5 Package, *The Journal of Chemical Physics*, 155(8) 2021
10. J.-Y. Yeh;S.-C. Li;C. H. Chen;K. C.-W. Wu;Y.-P. Li, Quantum Mechanical Calculations for Biomass Valorization over Metal-Organic Frameworks (MOFs), *Chemistry – An Asian Journal* , 16(9) 2021
 11. K. Ahuja;W. H. Green;Y.-P. Li, Learning to Optimize Molecular Geometries Using Reinforcement Learning, *Journal of Chemical Theory and Computation*, 17(2)818-825-2021J.-Y. Yeh;B. M. Matsagar;S. S. Chen;H.-L. Sung;D. C. W. Tsang;Y.-P. Li;K. C.-W. Wu, Synergistic effects of Pt-embedded, MIL-53-derived catalysts (Pt@Al₂O₃) and NaBH₄ for water-mediated hydrogenolysis of biomass-derived furfural to 1,5-pentanediol at near-ambient temperature, *Journal of Catalysis*, 390(4)46-56-202044036C. A. Grambow, **Y.-P. Li** and W. H. Green, "Accurate Thermochemistry with Small Data Sets: A Bond Additivity Correction and Transfer Learning Approach", *The Journal of Physical Chemistry A*, 123(27), 5826–5835, 2019(Jun)
 12. M. Keçeli, S. N. Elliott, **Y.-P. Li**, M. S. Johnson, C. Cavallotti, Y. Georgievskii, W. H. Green, M. Pelucchi, J. M. Wozniak and A. W. Jasper, "Automated computational thermochemistry for butane oxidation: A prelude to predictive automated combustion kinetics", *Proceedings of the Combustion Institute*, 37(1), 363-371, 2019(Aug).
 13. **Y.-P. Li**, K. Han, C. A. Grambow and W. H. Green, "Self-evolving machine: A continuously improving model for molecular thermochemistry", *The Journal of Physical Chemistry A*, 123(10), 2019(Feb).
 14. C. A. Grambow, A. Jamal, **Y.-P. Li**, W. H. Green, J. Zador and Y. V. Suleimanov, "Unimolecular reaction pathways of a γ -ketohydroperoxide from combined application of automated reaction discovery methods", *Journal of the American Chemical Society*, 140(3), 1035-1048, 2018(Dec).

Conference Papers

1. Yi-Pei Li, Explainable uncertainty quantifications for deep learning-based molecular property prediction, 2023 化學年會, Kaohsiung, Taiwan, 2023/3/10-3/12(Invited Speaker)
2. Yi-Pei Li, Deep Learning in Chemical Design and Property Prediction, 台積電專題演講, Online, 2022/12/8(Invited Speaker)
3. Lung-Yi Chen; Yi-Pei Li, Machine Learning Approach for Reaction Condition Recommendation, 台灣化學工程學會 69 週年年會, Taipei, Taiwan, 2022/12/2
4. Yen-Hsiang Lin; Hsin-Hao Liang; Shiang-Tai Lin; Yi-Pei Li, A Novel Vapor Pressure Prediction Model Using Deep Learning Algorithm, 台灣化學工程學會 69 週年年會, Taipei, Taiwan, 2022/12/2
5. Shih-Cheng Li; Yen-Chun Lin; Yi-Pei Li, Analysis of Uncoupled Mode Models in Gas Phase Reactions, 台灣化學工程學會 69 週年年會, Taipei, Taiwan, 2022/12/2
6. Shih-Cheng Li; Yen-Chun Lin; Yi-Pei Li, Analyzing the Performance of Uncoupled Mode Approximations in Reaction Rate Calculations, 2022 AIChE Annual Meeting, Phoenix, AZ, USA, 2022/11/13
7. Yi-Pei Li, The Good and the Bad of Deep Learning for Molecular Property Predictions, 理論與計算分子科學論壇, Online, 2022/10/27(Invited Speaker)
8. Jyun-Yi Yeh; Kevin C.-W. Wu; Yi-Pei Li, Theoretical Study of the Hydrogenolysis and Hydrodeoxygenation of Furfuryl Alcohol over Cobalt Single-Site Catalysts Anchored on Metal-Organic Frameworks, International Symposium on Porous Materials 2022, Tokyo, Japan, 2022/10/12(Invited Speaker)
9. Yi-Pei Li, Computer-Aided Mechanism Discovery and Reaction Engineering, 台大應力所專題演講, Taipei, Taiwan, 2022/9/26(Invited Speaker)
10. Shih-Cheng Li; Yen-Chun Lin; Yi-Pei Li, A Comparative Analysis of Uncoupled Mode Approximations in Gas Phase Reactions, 2022 台灣理論計算分子科學學會研討會, Taipei, Taiwan, 2022/9/3
11. Hsin-Yu Yu; Shih-Cheng Li; Yi-Pei Li, A Neural Network Model for Surface Characterization of Cerium Oxide Catalysts Based on Infrared Spectroscopy, 2022 台灣理論計算分子科學學會研討會, Taipei, Taiwan, 2022/9/3
12. Yen-Hsiang Lin; Yi-Pei Li, Deep Learning-Based Vapor Pressure Prediction, 2022 台灣理論計算分子科學學會研討會, Taipei, Taiwan, 2022/9/3
13. Lung-Yi Chen; Yi-Pei Li, Machine Learning Approach for Reaction Condition Recommendation, 2022 台灣理論計算分子科學學會研討會, Taipei, Taiwan, 4 2022/9/3

14. Tsai-Ho Li; Yi-Pei Li, An Analytical Approach for Deriving Rate Expressions of Complex Reaction Networks, Taipei International Conference on Catalysis (TICC-2022), Taipei, Taiwan, 2022/7/20
15. Hsin-Yu Yu; Shih-Cheng Li; Yi-Pei Li, Deep Learning Based Microstructure Characterization of Cerium Oxide Catalysts, Taipei International Conference on Catalysis (TICC-2022), Taipei, Taiwan, 2022/7/20
16. Shih-Cheng Li; Yen-Chun Lin; Yi-Pei Li, Effect of Mesoporosity and Extra-framework Aluminum Species on the Cracking Activity of Zeolite Y, Taipei International Conference on Catalysis (TICC-2022), Taipei, Taiwan, 2022/7/20
17. Yi-Pei Li, Computational Elucidation of the Transition State Shape Selectivity on Metal-Organic Frameworks, Taipei International Conference on Catalysis (TICC-2022), Taipei, Taiwan, 2022/7/20
18. **Yi-Pei Li**, Challenges and Opportunities for Machine Learning in Chemical Engineering, 聚合國際專題演講, Kaohsiung, Taiwan, 2022/3/3(Invited Speaker)
19. Kabir Ahuja; Yu-Cheng Chang; William H. Green; **Yi-Pei Li**, Reinforcement Learning Assisted Molecular Geometry Optimizations, 台灣化學工程學會 68 週年年會, Kaohsiung, Taiwan, 2022/1/6
20. Tsai-Ho Li; **Yi-Pei Li**, Monte Carlo Simulations of Silica Polymerization in the Synthesis of MFI and TON Zeolites, 台灣化學工程學會 68 週年年會, Kaohsiung, Taiwan, 2022/1/6
21. **Yi-Pei Li**, Theoretical Methods for Efficient Modeling of Reactions in Metal-Organic Frameworks, 17th Taiwan-Japan Joint Symposium on Catalysis, Online, 2021/12/3(Invited Speaker)
22. **Yi-Pei Li**, Tuning of zeolite catalysts: computer-aided mechanism discovery and catalysis engineering, The 9th Workshop on Next-Generation Utilization of Natural Gas, Online, 2021/11/20(Invited Speaker)
23. **Yi-Pei Li**, Development of Theoretical Methods for Efficient Modeling of Reactions in Porous Catalysts, International Symposium on Porous Materials 2021, Online, 2021/11/4(Invited Speaker)
24. Chih-Ning Tsai; Lung-Yi Chen; **Yi-Pei Li**; Tzu-En Lin, Prediction of wine quality based on their chemical compositions using machine learning techniques, 2021 International Conference on Smart Sensors (ICSS 2021), Online, 2021/10/14
25. Chu-I Yang; **Yi-Pei Li**, Atomic Uncertainty Quantifications in Molecular Property Predictions via Graph Convolutional Neural Networks, 2021 台灣理論計算分子科學學會研討會, Taipei, Taiwan, 2021/9/3
26. Jian-Yi Li; **Yi-Pei Li**, ARMD: Automated Reaction Mechanism Discovery— Application to Catalytic Reactions, 2021 台灣理論計算分子科學學會研討會, Taipei, Taiwan, 2021/9/3
27. Lung-Yi Chen; **Yi-Pei Li**, Machine Learning Approach for Reaction Condition

- Recommendation, 2021 熱力學暨程序系統工程研討會, Nantou, Taiwan, 2021/5/24
28. Shih-Cheng Li; Yen-Chun Lin; **Yi-Pei Li**, Comparative Study of Uncoupled Mode Approximation in Different Coordinate Systems for Rate Calculations, 2021 熱力學暨程序系統工程研討會, Nantou, Taiwan, 2021/5/24
 29. Yi-Cheng Shih; Lung-Yi Chen; **Yi-Pei Li**; Tzu-En Lin, Synthesis of CuO Nanoparticles to Study the Redox Reaction in Red Wine, 2021 International Conference on Smart Sensors, Taipei, Taiwan, 2021/7/5
 30. **Yi-Pei Li**, Challenges and Opportunities for Machine Learning in Reaction Engineering, 催化反應機制探討研討會, Taipei, Taiwan, 2020/12/18(Invited Speaker)
 31. **Yi-Pei Li**, Tuning of Catalysts for Biofuel Conversions: A Computer-Aided Approach, 成大化工專題演講, Tainan, Taiwan, 2020/12/11(Invited Speaker)
 32. **Yi-Pei Li**, Computer-Aided Reaction Engineering: Tuning of Catalysts for Biofuel Conversions, 台大化學專題演講, Taipei, Taiwan, 2020/11/26(Invited Speaker)
 33. **Yi-Pei Li**, Computer-Aided Mechanism Discovery and Reaction Engineering, 科盛科技專題演講, Hsinchu, Taiwan, 2020/11/17(Invited Speaker)
 34. **Yi-Pei Li**, Tuning of Zeolite Catalysts for Biofuel Conversions: A Computer-Aided Approach, International Symposium on Porous Materials 2020, Taipei, Taiwan, 2020/11/6(Invited Speaker)
 35. Chu-I Yang; **Yi-Pei Li**, Understanding Uncertainties in Deep Learning for Molecular Property Predictions, 2020 台灣化學工程學會 67 週年年會&台日韓捷永續化學工程國際研討會, Hsinchu, Taiwan, 2020/10/23
 36. Shih-Cheng Li; **Yi-Pei Li**, Kinetics of Anharmonic Systems: Uncoupled Mode Approximations for Reaction Rate Estimations, 2020 台灣化學工程學會 67 週年年會&台日韓捷永續化學工程國際研討會, Hsinchu, Taiwan, 2020/10/23
 37. **Yi-Pei Li**, Computer-Aided Reaction Engineering: Tuning of Catalysts for Biofuel Conversions, 逢甲化工系專題演講, Taichung, Taiwan, 2020/10/19 (Invited Speaker)
 38. **Yi-Pei Li**, Computer-Aided Reaction Mechanism Discovery and Catalysis Engineering, 成大化學系專題演講, Tainan, Taiwan, 2020/9/29(Invited Speaker)
 39. **Yi-Pei Li**, Challenges and Opportunities for Machine Learning in Reaction Engineering, 2020 台灣化學產業高峰論壇, Taipei, Taiwan, 2020/9/1(Invited Speaker)
 40. Tsai-Chen Hsiung; Ting-Wei Hsu; **Yi-Pei Li**, Range-Separated Fingerprints for Improved Molecular Representations, 2020 台灣理論計算分子科學學會研討會, Taipei, Taiwan, 2020/8/6

41. Ting-Wei Hsu; Tsai-Chen Hsiung; **Yi-Pei Li**, An Improved Machine Learning Model for the Prediction of Heat of Formation, 2020 台灣理論計算分子科學學會研討會, Taipei, Taiwan, 2020/8/6
42. **Yi-Pei Li**, Deep Learning for Accurate Thermochemistry Predictions, 第三十八屆台灣觸媒及反應工程研討會, Taipei, Taiwan, 2020/7/16(Invited Speaker)
43. **Yi-Pei Li**, Computer-Aided Mechanism Discovery and Reaction Engineering, 2020 化學與材料模擬暨產業應用論壇, Hsinchu, Taiwan, 2020/6/18(Invited Speaker)
44. **Yi-Pei Li**, Computer-Aided Reaction Engineering:Tuning of Catalysts for Biofuel Conversions, 中央化材系專題演講, Taoyuan, Taiwan, 2020/3/27(Invited Speaker)
45. **Yi-Pei Li**, Computer-Aided Reaction Engineering:Tuning of Catalysts for Biofuel Conversions, 清大化工系專題演講, Hsinchu, Taiwan, 2020/3/18(Invited Speaker)
46. **Yi-Pei Li**, "Towards High Fidelity Reaction Modeling by Combining Quantum Mechanics and Machine Learning", 第八屆海峽兩岸理論計算化學研討會, Taipei, Taiwan, 2019(Dec), **Invited Speaker and Session Chair**
47. **Yi-Pei Li**, Kehang Han, Colin A. Grambow and William H. Green, "Towards High Fidelity Reaction Modeling by Combining Quantum Mechanics and Machine Learning", 2019 台灣化學工程學會 66 週年年會, Taichung, Taiwan, 2019(Nov), **Invited Speaker**
48. Ting-Wei Hsu, Ke-Yang Dai, Kehang Han, Colin A. Grambow, William H. Green and **Yi-Pei Li**, "Uncertainty Quantification for Machine Learning and a Self-Learning Model for Molecular Property Prediction", 2019 台灣化學工程學會 66 週年年會, Taichung, Taiwan, 2019(Nov)
49. Tsai-Chen Hsiung, Colin A. Grambow, William H. Green and **Yi-Pei Li**, "Machine Learning with Small Data Sets for Molecular Property Prediction", 2019 台灣化學工程學會 66 週年年會, Taichung, Taiwan, 2019(Nov)
50. **Yi-Pei Li**, "Application of Quantum Mechanics and Machine Learning in Reaction Engineering", Seminar at the College of Chemistry and Chemical Engineering, Fuzhou University, Fuzhou, China, 2019(Nov), **Invited Speaker**
51. **Yi-Pei Li**, "Computer-Aided Reaction Mechanism Discovery and Catalysis Engineering", Seminar at the Department of Chemical and Materials Engineering, University of Alberta, Edmonton, AB, Canada, 2019(Apr), **Invited Speaker**
52. **Yi-Pei Li**, "Engineering Chemical Reactions with Quantum Mechanics and Machine Learning", Seminar at the Department of Mineral and Energy Engineering, Penn State University, University Park, PA, USA, 2019(Apr), **Invited Speaker**
53. **Yi-Pei Li**, Kehang Han, Colin A. Grambow and William H. Green, "Self-Evolving Machine: A Continuously Improved Model for Molecular Thermochemistry", 256th ACS National Meeting, Boston, MA, USA, 2018(Aug)

54. **Yi-Pei Li**, "Computer-Aided Reaction Engineering: Tuning of Catalysts for Biofuel Conversions", Seminar at the Academia Sinica, Taipei, Taiwan, 2018(Apr), **Invited Speaker**
55. Colin A. Grambow, Adeel Jamal, **Yi-Pei Li**, William H. Green, Judit Zádor and Yury V. Suleimanov, "Automated Reaction Discovery from Combined Application of Transition State Search Algorithms", 2018 APS Meeting, Los Angeles, CA, USA, 2018(Mar)
56. **Yi-Pei Li**, "Computer-Aided Reaction Engineering: Tuning of Catalysts for Biofuel Conversions", Seminar at the Department of Chemical Engineering, Texas A&M, College Station, TX, USA, 2018(Feb), **Invited Speaker**
57. **Yi-Pei Li**, Kehang Han and William H. Green, "Estimation of Thermodynamic Properties of Polycyclic Molecules by a Linear Regression Model", 2017 AIChE Annual Meeting, Minneapolis, MN, USA, 2017(Oct)

Honors and Others

1. 指導專題生張平同學參與本系「大學專題海報競賽」並獲得佳作 (2022)
2. 指導專題生陳景淳同學參與本系「大學專題海報競賽」並獲得佳作 (2022)
3. 指導實驗室博士生李世晟同學獲得義芳化學鼓勵優秀博士生獎學金 (2021)
4. 指導實驗室博士生陳隆奕同學於 2021 International Conference on Smart Sensors 獲得 Distinguished Award (2021)
5. 指導實驗室博士生陳隆奕同學獲得台大校長獎 (2021)
6. 指導實驗室碩士生楊筑宜同學於台灣理論計算分子科學學會獲得最佳中文報告獎 (2021)
7. 指導實驗室碩士生陳隆奕同學於熱力學暨程序系統工程研討會(線上會議)獲得最多觀看報告獎 (2021)
8. 指導實驗室碩士生李建毅同學榮獲「松柏優秀化工產品開發競賽佳作」 (2021)
9. 指導實驗室碩士生李建毅同學榮獲「長春集團傑出論文獎」 (2021)
10. 指導實驗室碩士生李建毅同學榮獲「達興傑出論文獎」 (2021)
11. 指導實驗室博士生葉俊毅同學中央研究院 AS-TIGP presidential Fellowship (2020)
12. 指導實驗室博士生李世晟同學獲得台大校長獎 (2020)
13. 指導實驗室專題生熊才誠同學於台灣理論計算分子科學學會獲得最佳壁報獎 (2020)

14. 指導實驗室碩士生許鼎威同學於台灣理論計算分子科學學會獲得最佳中文報告獎 (2020)
15. 指導研究室專題生熊才誠同學參與本系「大學專題海報競賽」並獲得銅獎 (2020)
16. 指導研究室碩士生李世晟同學與堉璘宏泰基金會合作·為台灣未來可能面臨的社會問題規劃解決方案·該生於 109 年獲得該基金會之「堉璘獎學金」 (2019)
17. 機器學習研究成果受到國際肯定·獲選為美國國家能源研究科學計算中心 NERSC Science Highlight (2019)
18. Outstanding Scholar Award, Foundation for the Advancement of Outstanding Scholarship, Taiwan (2019)

