Lin, Shiang-Tai（林祥泰）
Professor

B.S. in Chemical Engineering
National Taiwan University, 1994
Ph.D. in Chemical Engineering
University of Delaware, 2000

Research and Professional Interests
Applied Computational Chemistry
Statistical Thermodynamics
Renewable Energy

Journal Papers

1. **B.-Y. Yu**, P.-J. Wu, C.-C. Tsai, and S.-T. Lin, Production of diethyl carbonate from direct CO2 conversion. In *Chemical Engineering Process Simulation*, Foo, D. C. Y., Ed. Elsevier: 2023; pp 391-424.

2. N. Venkatareddy, S.-T. Lin, and **P. K. Maiti**, Phase behavior of active and passive dumbbells. *PHYSICAL REVIEW E* 107, 034607, 2023.

3. C. C. Tsai, A. McNeeley, S. T. Lin, and **Y. A. Liu**, Evaluation of thermophysical data, COSMO-SAC predictions, and feed simplifications for aromatic extraction process simulation using ionic liquid EMIM NTf2. *AIChE J.*, 69 (2), e17916, 2023.

4. C. C. Tsai, and **S. T. Lin**, Improved vapor pressure prediction from PR plus COSMOSAC EOS using normal boiling temperature. *AIChE J.*, 69 (3), e17997, 2023.

5. S. Naskar, D. Bhatia, S. T. Lin, and **P. K. Maiti**, Mechanistic insight into the structure, thermodynamics and dynamics of equilibrium gels of multi-armed DNA nanostars. *Phys. Chem. Chem. Phys.*, 25 (11), 7847-7858, 2023.

6. A. McNeeley, C. C. Tsai, S. T. Lin, and **Y. A. Liu**, Science-guided data analytics for selecting ionic liquid solvents for aromatic extraction. *AIChE J.*, e18081, 2023.

7. A. McNeeley, C. C. Tsai, S. T. Lin, and **Y. A. Liu**, Development of energy-optimum aromatic extraction processes using ionic liquid EMIM NTf2. *AIChE J.*, 69 (2), e17888, 2023.

8. Y. C. Hung, C. M. Hsieh, H. Machida, S. T. Lin, and **Y. Shimoyama**, Modeling of phase separation solvent for CO2 capture using COSMO-SAC model. *Journal of the Taiwan Institute of Chemical Engineers*, 135, 104362, 2022.

9. Y. C. Hung, C. M. Hsieh, H. Machida, S. T. Lin, and **Y. Shimoyama**, Unveiling the mechanism of CO2-driven phase change in amine plus water plus glycol ether ternary mixture. *Journal of the Taiwan Institute of Chemical Engineers*, 131, 104143, 2022.

10. Y. Hung, C. Hsieh, H. Machida, S. Lin, and **Y. Shimoyama**, Phase Equilibrium Modeling of Mixtures Containing Conformationally Flexible Molecules with the COSMO-SAC Model. *Journal of Molecular Liquids*, 356, 118896, 2022.

11. P. W. Wang, D. T. Wu, and **S. T. Lin**, Promotion mechanism for the growth of CO2 hydrate with urea using molecular dynamics simulations. *Chemical Communications*, 57, 5330-5333, 2021.

12. T. Vikramaditya, and **S. T. Lin**, Novel Donor-Electret-Acceptor Framework for Higher Charge Transfer and Distance of Charge Transfer through Dipole Engineering. *J. Phys. Chem. C*, 125 (37), 20219-20229, 2021.

13. C. T. Lee, C. C. Tsai, P. J. Wu, **B. Y. Yu**, and **S. T. Lin**, Screening of CO2 utilization routes from process simulation: Design, optimization, environmental and techno-economic analysis. *Journal of Co2 Utilization*, 53, 101722, 2021.

14. Y.-C. Hung, C.-M. Hsieh, H. Machida, S.-T. Lin, and **Y. Shimoyama**, Towards Design of Phase Separation Solvent for CO2 Capture using COSMO-SAC Model. *Journal of Molecular Liquids*, 336, 116229, 2021.

15. J. J. Chang, **D. S. H. Wong**, C. H. Huang, J. L. Kang, H. H. Hsu, and S. T. Lin, Towards a universal digital chemical space for pure component properties prediction. *Fluid Phase Equilib.*, 527, 112829, 2021.

16. **B.-Y. Yu**, P.-J. Wu, C.-C. Tsai, and **S.-T. Lin**, Evaluating the direct CO2 to diethyl carbonate (DEC) process: Rigorous simulation, techno-economical and environmental evaluation. *Journal of CO2 Utilization*, 41, 101254, 2020.

17. T. Vikramaditya, and **S.-T. Lin**, Accurate Prediction of Vertical Emission from Excited-State Tuning of Range-Separated Density Functional Theory. *J. Phys. Chem. C*, 2020.

18. C. C. Tsai, and **S. T. Lin**, Integration of Modern Computational Chemistry and ASPEN PLUS for Chemical Process Design. *AIChE J.*, 66 (10), e16987, 2020.

19. K.-Y. Chang, C.-K. Chu, L.-S. Chu, Y.-A. Chen, S.-T. Lin, Y.-P. Chen, and **L.-J. Chen**, Effect of Small Cage Guests on Dissociation Properties of Tetrahydrofuran Hydrates. *J. Phys. Chem. B*, accepted, 2020.

20. C.-K. Chang, and **S.-T. Lin**, Improved Prediction of Phase Behaviors of Ionic Liquid Solutions with Consideration of Directional Hydrogen Bonding Interactions. *Ind. Eng. Chem. Res.*, 59, 3550−3559, 2020.

21. C. K. Chang, and **S. T. Lin**, Extended Pitzer–Debye–Hückel Model for Long-Range Interactions in Ionic Liquids. *J. Chem. Eng. Data*, 65 (3), 1019-1027, 2020.

22. Z.-Z. Cai, H.-H. Liang, W.-L. Chen, S.-T. Lin, and **C.-M. Hsieh**, First-principles prediction of solid solute solubility in supercritical carbon dioxide using PR+ COSMOSAC EOS. *Fluid Phase Equilib.*, 522, 112755, 2020.

23. **I. H. Bell**, E. Mickoleit, C.-M. Hsieh, S.-T. Lin, J. Vrabec, C. Breitkopf, and A. Jäger, A Benchmark Open-Source Implementation of COSMO-SAC. *J. Chem. Theory Comput.*, 16 (4), 2635–2646, 2020.

24. T. Vikramaditya, and **S. T. Lin**, Limitations of Global Hybrids in Predicting the Geometries and Torsional Energy Barriers of Dimeric Systems and the Role of Hartree Fock and DFT Exchange. *J. Comput. Chem.*, 40 (32), 2810-2818, 2019.

25. Y.-R. Tsai, and **S.-T. Lin**, Prediction and Reasoning for the Occurrence of Lower Critical Solution Temperature in Aqueous Solution of Ionic Liquids. *Ind. Eng. Chem. Res.*, 58, 10064−10072, 2019.

26. S. S. P. Sivajothi, S.-T. Lin, and **P. K. Maiti**, Efficient Computation of Entropy and Other Thermodynamic Properties for Two-Dimensional Systems Using Two-Phase Thermodynamic Model. *J. Phys. Chem. B*, 123 (1), 180-193, 2019.

27. T.-C. Liu, and **S.-T. Lin**, Exact Local Composition Model for Two-Dimensional Lattice Fluids. *Ind. Eng. Chem. Res.*, 58 (45), 20779-20787, 2019.

28. T.-C. Liu, and **S.-T. Lin**, A new approach for developing exact local composition models for lattice fluids. *Journal of the Taiwan Institute of Chemical Engineers*, 96, 63-73, 2019.

29. H. H. Liang, J. Y. Li, L. H. Wang, S. T. Lin, and **C. M. Hsieh**, Improvement to PR plus COSMOSAC EOS for Predicting the Vapor Pressure of Nonelectrolyte Organic Solids and Liquids. *Ind. Eng. Chem. Res.*, 58 (12), 5030-5040, 2019.

30. C. H. Li, C. C. Tsai, M. Y. Liao, Y. A. Su, S. T. Lin, and **C. C. Chueh**, Stable, color-tunable 2D SCN-based perovskites: revealing the critical influence of an asymmetric pseudo-halide on constituent ions. *Nanoscale*, 11 (6), 2608-2616, 2019.

31. H. H. Hsu, C. H. Huang, and **S. T. Lin**, New Data Structure for Computational Molecular Design with Atomic or Fragment Resolution. *Journal of Chemical Information and Modeling*, 59 (9), 3703-3713, 2019.

32. L. S. Chu, **D. T. Wu**, and **S. T. Lin**, Theory and Kinetic Monte Carlo Simulation of Guest Molecule Transport in sI Clathrate Hydrates Based on Cage Hopping. *J. Phys. Chem. C*, 123 (17), 11233-11243, 2019.

33. L. H. Wang, C. M. Hsieh, and **S. T. Lin**, Prediction of Gas and Liquid Solubility in Organic Polymers Based on the PR plus COSMOSAC Equation of State. *Ind. Eng. Chem. Res.*, 57 (31), 10628-10639, 2018.

34. **J. Vrabec**, M. Bernreuther, H. J. Bungartz, W. L. Chen, W. Cordes, R. Fingerhut, C. W. Glass, J. Gmehling, R. Hamburger, M. Heilig, M. Heinen, M. T. Horsch, C. M. Hsieh, M. Hulsmann, P. Jager, P. Klein, S. Knauer, T. Koddermann, A. Koster, K. Langenbach, S. T. Lin, P. Neumann, J. Rarey, D. Reith, G. Rutkai, M. Schappals, M. Schenk, A. Schedemann, M. Schonherr, S. Seckler, S. Stephan, K. Stobener, N. Tchipev, A. Wafai, S. Werth, and H. Hasse, SkaSim - Scalable HPC Software for Molecular Simulation in the Chemical Industry. *Chem. Ing. Tech.*, 90 (3), 295-306, 2018.

35. T. Vikramaditya, **J. D. Chai**, and **S. T. Lin**, Impact of non-empirically tuning the range-separation parameter of long-range corrected hybrid functionals on ionization potentials, electron affinities, and fundamental gaps. *J. Comput. Chem.*, 39 (28), 2378-2384, 2018.

36. Z.-Y. Lin, **D. T. Wu**, and **S.-T. Lin**, Equilibrium and Transport Properties of Methane at the Methane/Water Interface with the Presence of SDS. *J. Phys. Chem. C*, 122, 29259−29267, 2018.

37. H. H. Hsu, C. H. Huang, and **S. T. Lin**, Fully Automated Molecular Design with Atomic Resolution for Desired Thermophysical Properties. *Ind. Eng. Chem. Res.*, 57 (29), 9683-9692, 2018.

38. Y. A. Chen, C. K. Chu, Y. P. Chen, L. S. Chu, S. T. Lin, and **L. J. Chen**, Measurements of diffusion coefficient of methane in water/brine under high pressure. *Terr. Atmos. Ocean. Sci.*, 29 (5), 577-587, 2018.

39. C. Y. Chen, L. H. Wang, **C. M. Hsieh**, and S. T. Lin, Prediction of solid-liquid-gas equilibrium for binary mixtures of carbon dioxide plus organic compounds from approaches based on the COSMO-SAC model. *J. Supercrit. Fluids*, 133, 318-329, 2018.

40. C. K. Chang, W. L. Chen, D. T. Wu, and **S. T. Lin**, Improved Directional Hydrogen Bonding Interactions for the Prediction of Activity Coefficients with COSMO-SAC. *Ind. Eng. Chem. Res.*, 57 (32), 11229-11238, 2018.

Conference Papers

1. 黃晨軒, and S.-T. Lin, Implementation of Computer-Aided Molecular Design via

MARS-PLUS Package. In *台灣化學工程學會 68 週年年會*, 高雄展覽館三樓, 2022.

2. 蔡昌哲, and S.-T. Lin, Improved Prediction of Vapor Pressure from PR+COSMOSAC EOS with Normal Boiling Point. In *台灣化學工程學會 68 週年年會*, 高雄展覽館三樓, 2022.

3. 梁興豪, and S.-T. Lin, Accuracy of PR+COSMOSAC EOS in Predicting Vapor Pressure with Machine Learning. In *台灣化學工程學會 68 週年年會*, 高雄展覽館三樓, 2022.

4. 施彥任, and S.-T. Lin, Liquid-Liquid Equilibrium Prediction from COSMOSAC Model with Global Renormalization Group Theory. In *台灣化學工程學會 68 週年年會*, 高雄展覽館三樓, 2022.

5. P.-W. Wang, D. T. Wu, and S.-T. Lin, Revealing the Mechanism for Promotion of Gas Hydrate Growth using Chemical Additives. In *台灣化學工程學會 68 週年年會*, 高雄展覽館三樓, 2022.

6. H.-L. Wen, and S.-T. Lin, Thermodynamic Properties of Fluids from Artificial Neural Network. In *2021 Symposium on Thermodynamics and Process Systems Engineering*, 台灣大學(virtual), 2021.

7. T. Vikramaditya, and S.-T. Lin, Prediction of Accurate Vertical Emission Energies from the Excited State Tuning of Range Separated Density Functional Theory. In *2021 化學會年會*, 國立中央大學, 2021.

8. T. Vikramaditya, and S.-T. Lin, High Charge Transfer and Charge Separation Donor-Electret-Acceptor Framework for Solar Cell Applications. In *2021 AIChE Annual Meeting*, Boston (virtual), USA, 2021.

9. C.-C. Tsai, and S.-T. Lin, Prediction of vapor pressure of large and chemically diverse dataset using PR+COSMOSAC EOS. In *2021 Symposium on Thermodynamics and Process Systems Engineering*, 台灣大學(virtual), 2021.

10. A. Sum, L. Wang, and S.-T. Lin, A New Approach for Correlating the Solution Properties of Strong Electrolyte Systems. In *31st European Symposium on Applied Thermodynamics*, France (virtual), 2021.

11. T.-C. Liu, and S.-T. Lin, COSMO-SAC: a Reliable Predictive Model for Thermodynamic Properties of Liquid Mixtures. In *2021 Symposium on Thermodynamics and Process Systems Engineering*, 台灣大學(virtual), 2021.

12. S.-T. Lin, C.-M. Hsieh, C.-C. Tsai, and C.-H. Huang, Improvements on the Predictive COSMO-SAC Model and its Applications in Process and Product Design. In *The 9th international symposium on Molecular Thermodynamics and Molecular Simulation*, Japan (virtual), 2021.

13. D. Kumar, and S.-T. Lin, sII-Hydrate Nucleation in the Presence of Ice Interface: A Molecular Dynamics Study. In *2020 Annual Meeting of the Society of Interface Science*, National Taiwan University (virtual), 2021.

14. D. Kumar, and S.-T. Lin, Propane-Hydrate Nucleation in the Presence of Ice Interface: A Molecular Dynamics Study. In *2021 AIChE Annual Meeting*, Boston (virtual), USA, 2021.

15. Y.-C. Hung, C.-M. Hsieh, H. Machida, S.-T. Lin, and Y. Shimoyama, Liquid-Liquid Equilibrium Prediction of Mixtures Containing Alkylene Glycol Derivatives from COSMO-SAC with Conformational Information. In *SCEJ 52nd Autumn Meeting*, Okayama University, Japan, 2021.

16. C.-H. Huang, and S.-T. Lin, Computer-Aided Molecular Design and Its Applications on the Integrated Solvent-Process Design. In *2021 Symposium on Thermodynamics and Process Systems Engineering*, 台灣大學(virtual), 2021.

17. F. Chen, and S.-T. Lin, Computer Simulation of Sugar Alcohols as Phase-Change Materiasls (PCMs). In *2021 Symposium on Thermodynamics and Process Systems Engineering*, 台灣大學(virtual), 2021.

18. B.-Y. Yu, P.-J. Wu, C.-C. Tsai, and S.-T. Lin, Evaluating the Direct CO2 to Diethyl Carbonate (DEC) Process: Rigorous Simulation, Techno-Economical and Environmental Evaluation. In *The 9th PSE Asia*, National Taiwan University (virtual), 2020.

19. C.-C. Tsai, P.-J. Wu, B.-Y. Yu, and S.-T. Lin, Thermophysical properties Estimation for Aspen Plus Modeling. In *台灣化學工程學會第67屆年會*, 清華大學, 2020.

20. C.-C. Tsai, and S.-T. Lin, Process Design with ASPEN PLUS when Some or All Experimental Data are not Available. In *The 9th PSE Asia*, National Taiwan University (virtual), 2020.

21. Y.-J. Shih, and S.-T. Lin, Improvement of LLE Prediction from COSMO-SAC Near Critical Point using Transformation of Variables and Renormalization Group Theory. In *台灣化學工程學會第67屆年會*, 清華大學, 2020.

22. D. Kumar, D. T. W. Wu, and S.-T. Lin, Inhibition of Ice growth and quick CH4 Hydrate Nucleation: A Molecular Dynamics Study. In *台灣化學工程學會第67屆年會*, 清華大學, 2020.

23. D. Kumar, D. T. W. Wu, and S.-T. Lin, Methane Hydrate Nucleation Mechanism in the Presence of Growing Ice Front: A Molecular Dynamics Simulation Study. In *台灣化學工程學會第67屆年會*, 清華大學, 2020.

24. D. Kumar, and S.-T. Lin, Methane Hydrate Nucleation Mechanism in the Presence of Growing Ice Front: A Molecular Dynamics Simulation Study. In *台灣化學工程學會第67屆年會*, 清華大學, 2020.

25. D. Kumar, and S.-T. Lin, Promoting CH4 hydrate Nucleation in the presence of Ice : A Molecular Dynamics Study. In *2020 Annual Meeting of the Society of Interface Science*, National Taiwan University, 2020.

26. Y.-C. Hung, C.-M. Hsieh, H. Machida, S.-T. Lin, and Y. Shimoyama, Molecular Design and Development of Phase-Separation Solvent for CO2 Capture Using COSMO-SAC Model. In *The Society of Chemical Engineers Japan, 51 Autumn Meeting*, Iwate University (virtual), Japan, 2020.

27. C.-H. Huang, and S.-T. Lin, Computer-Aided Molecular Design for Chemical and Energy Applications. In *2020 AIChE Annual Meeting*, San Francisco (virtual), USA, 2020.

28. 黃晨軒, and 林祥泰, Fully Automated Molecular Design with Atomic Resolution for Desired Thermophysical Properties. In *台灣化學工程學會第 66 屆年會*, 東海大學, 2019.

29. 王柏偉, and 林祥泰, Molecular Dynamics Simulation Study on the Effect of Urea to the Equlibrium and Kinetic Properties of Methane and CO2 Hydrates. In *台灣化學工程學會第66屆年會*, 東海大學, 2019.

30. 林祥泰, 分子模擬與人工智慧在化學工程上的應用. In *數位管理x研發創新跨界論壇*, 台北寒舍艾美酒店, 2019.

31. 李政廷, and 林祥泰, A Unified Model for the Activity Coefficient of Electrolyte and Nonelectrolyte Solutions. In *台灣化學工程學會第66屆年會*, 東海大學, 2019.

32. 劉德謙, and 林祥泰, An Exact Local Composition Model for Two-Dimensional Lattice Fluids. In *台灣化學工程學會第66屆年會*, 東海大學, 2019.

33. C.-C. Tsai, B.-Y. Yu, and S.-T. Lin, A Novel Way to Perform Process Design with Missing Thermodynamic Parameters. In *2019 Symposium on Process Systems Engineering*, Xitou Nature Education Area, 2019.

34. C.-C. Tsai, and S.-T. Lin, Process Design with ASPEN PLUS when Some or All Experimental Data are not Available. In *台灣化學工程學會第66屆年會*, 東海大學, 2019.

35. V. Talapunur, and S.-T. Lina, Understanding the Role of Hartree-Fock and DFT Exchange in Altering Torsional Energies and Molecular Geometries. In *The 18th Asian Chemical Congress*, Taipei, 2019.

36. A. Sum, and S.-T. Lin, Developing of a Universal Activity Correlation for Strong Electrolyte Systems. In *International Conference on Properties and Phase Equilibria for Product and Process Design*, Vancouver, Canada, 2019.

37. T.-C. Liu, and S.-T. Lin, Exact Local Composition Model for Two-Dimensional Lattice Fluids. In *2019 Symposium on Process Systems Engineering*, Xitou Nature Education Area, 2019.

38. H.-F. Liu, and S.-T. Lin, Heat Capacity of Liquids from Classical Molecular Dynamic Simulations and the Two-Phase Thermodynamic Model. In *台灣化學工程學會第66屆年會*, 東海大學, 2019.

39. H.-F. Liu, and S.-T. Lin, Quantum Corrections to Heat Capacity of Liquids from Classical Molecular Dynamic Simulations and the Two-Phase Thermodynamic Model. In *The 5th International Conference on Molecular Simulation*, Lotte Hotel Jeju, Jeju, Korea, 2019.

40. S.-T. Lin, A Priori Prediction of Thermodynamic Properties and Phase Behaviors of

Fluids and Its Applications. In *台灣化學工程學會第66屆年會*, 東海大學, 2019.

41. H.-H. Liang, C.-M. Hsieh, and S.-T. Lin, Accuracy of PR+COSMOSAC EOS in Predicting Vapor Pressure with Artificial Neural Network. In *台灣化學工程學會第66屆年會*, 東海大學, 2019.

42. Jie-JiunChang, J.-L. Kang, D. S.-H. lWong, C.-H. Chou, H.-H. Hsu, C.-H. Huang, and S.-T. Lin In *Machine Learning of Molecular Classification and Quantum Mechanical Calculations*, 29th European Symposium on Computer Aided Process Engineering, Eindhoven, The Netherlands, Jun 16-19, 2019; Kiss, A. A.; Zondervan, E.; Lakerveld, R.; Özkan, L., Eds. Elsevier: Eindhoven, The Netherlands, 2019; pp 787-792.

43. H.-H. Hsu, C.-H. Huang, and S.-T. Lin, Fully Automated Molecular Design for Specialty Chemicals. In *The 5th International Conference on Molecular Simulation*, Lotte Hotel Jeju, Jeju, Korea, 2019.

44. Y.-H. Ho, and S.-T. Lin, Interfacial Properties of Methane Hydrate and Water via Molecular Dynamics Simulations. In *2019 Symposium on Process Systems Engineering*, Xitou Nature Education Area, 2019.

45. T. Ya-Ruei, H. Chiung-Hui, and S.-T. Lin, Prediction of phase behaviors of LCST-type ionic liquids in aqueous solution based on COSMO-SAC model. In *2018 熱力學暨程序系統工程研討會議程*, 成功大學化工系館, 2018.

46. C.-C. Tsai, and S.-T. Lin, A Novel Approach for Process Design When Some or All Experimental Thermodynamic Data are Missing. In *6th International Symposium on Processes Intensification*, NTU, Taipei, 2018.

47. A. Sum, and S.-T. Lin, Developing of a Universal Activity Correlation for Strong Electrolyte Systems. In *TWENTIETH SYMPOSIUM ON THERMOPHYSICAL PROPERTIES*, Boulder, CO, USA, 2018.

48. A. Sum, and S.-T. Lin, Developing of a Universal Activity Correlation for Strong Electrolyte Systems. In *2018 AIChE Annual Meeting*, Pittsburg, USA, 2018.

49. Z.-Y. Lin, D. Wu, and S.-T. Lin, Equilibrium and Transport Properties of Methane at the Methane-Water Interface with the Presence of SDS. In *台灣化學工程學會第65屆年會*, 雲林科技大學, 2018.

50. Z.-Y. Lin, and S.-T. Lin, The Promotion of Gas Hydrate Formation Upon Addition of Sodium Dodecyl Sulfate: A Molecular Dynamics Simulation Study. In *台灣化學工程學會第65屆年會*, 雲林科技大學, 2018.

51. S.-T. Lin, 預測固體溶質於超臨界二氧化碳之溶解度. In *第十七屆超臨界流體技術應用與發展研討會*, 明志科技大學, 2018.

52. S.-T. Lin, The Two-Phase Thermodynamic Approach for Absolute Entropy and Free Energy from Molecular Dynamics Simulations. In *Recent Advances in Molecular Simulations*, Indian Institute of Science, Bangalore, 2018.

53. S.-T. Lin, Introduction to the Two-Phase Thermodynamic Approach for Obtaining Absolute Entropy and Free Energy from Molecular Dynamics Simulations. In *Soft Matter Winter School at Institute of Physics*, Academia Sinica, 2018.

54. H.-E. Lai, and S.-T. Lin, Prediction of Vapor-Liquid Interfacial Tension of Fluids Using the Peng-Robinson Equation of State and Excess Free Energy based Mixing Rules. In *台灣化學工程學會第 65 屆年會*, 雲林科技大學, 2018.

55. H.-H. Hsu, C.-H. Huang, and S.-T. Lin, Fully Automated Molecular Design with Atomic Resolution for Desired ThermophysicalProperties. In *2018 熱力學暨程序系統工程研討會議程*, 成功大學化工系館, 2018.

56. H.-H. Hsu, C.-H. Huang, and S.-T. Lin, Fully Automated Molecular Design with Atomic Resolution for Desired Properties. In *2018 AIChE Annual Meeting*, Pittsburg, USA, 2018.

57. L.-S. Chu, D. T. Wu, and S.-T. Lin, Diffusion of Methane in sI Hydrates: A Kinetic Monte Carlo and Theoretical Study. In *2018 AIChE Annual Meeting*, Pittsburg, USA, 2018.

58. C.-K. Chang, W.-L. Chen, D. T. Wu, and S.-T. Lin, A Novel Approach for the Determination of Directional Hydrogen Bonding Interactions for the COSMO-SAC Model based on Molecular Electrostatic Potentials. In *2018 AIChE Annual Meeting*, Pittsburg, USA, 2018.

Book Chapter

1. B.-Y. Yu, P.-J. Wu, C.-C. Tsai, and S.-T. Lin, Production of diethyl carbonate from direct CO2 conversion. In *Chemical Engineering Process Simulation*, Foo, D. C. Y., Ed. Elsevier: 2023; pp 391-424.
2. M.-H. Lin, and S.-T. Lin, A Robust and Automated Approach for the Calculation of Absolute Entropy from the Two-Phase Thermodynamic Model with Gaussian Memory Function. In *Computational Materials, Chemistry, and Biochemistry: From Bold Initiatives to the Last Mile*, Shankar, S.; Muller, R.; Dunning, T.; Chen, G. H., Eds. Springer: 2021; pp 89-114.
3. S. T. Lin, and C. M. Hsieh, *Obtaining Thermodynamic Properties and Fluid Phase Equilibria without Experimental Measurements*. Intech: 2011; p 459-482.

Honors and Others

1. 指導學生呂紹維獲台大第四屆「學士班學生論文獎」傅斯年獎(2020)

2. 指導學生呂紹維獲台大化工 108 學年度學士專題海報競賽訊聯金獎(2020)

3. 指導學生陳奕安獲台大化工 108 學年度學士專題海報競賽銀獎(2020)

4. 指導學生古岱力，獲選參加 2020 灣化學工程學會 67 年年會英語口頭報告競賽論文競賽優等。

5. 指導學生蔡昌哲同學，獲得 2019 年台灣化學工程學會 66 週年年會壁報論文競賽-輸送組優勝

6. 指導學生劉曉丰同學，獲得 2019 年台灣化學工程學會 66 週年年會壁報論文競賽

-熱力及界面工程組優勝

7. 指導學生梁興豪同學，獲得 2019 年台灣化學工程學會 66 週年年會壁報論文競賽-熱力及界面工程組優勝

8. 指導學生林姿妤同學，獲科技部 107 年度大專生研究計畫創作獎 (2019)

9. 指導學生張峻愷同學，獲達興材料第八屆研究生獎學金 (2019)

10. 指導學生林姿妤同學，獲 2018 年台灣化學工程學會 65 週年年會英語口頭報告競賽論文競賽佳作

11. 指導學生林姿妤同學，獲得 2018 年台灣化學工程學會 65 週年年會壁報論文競賽-熱力及界面工程組佳作

12. 指導學生許軒豪與黃晨軒獲台大化工系 106 學年度學士專題競賽金牌 (2018)

13. 指導學生黃晨軒獲台大 106 學年度學士班學生論文院長獎 (2018)

14. 台灣大學 105 學年度教學傑出教師 (2017)

15. 指導學生張峻愷同學，獲科技部 105 年度大專生研究計畫創作獎 (2017)

16. 論文被 Physical Chemistry Chemical Physics 選為期刊封底(2017)

17. 指導學生陳威霖，獲得 2016 達興材料博士班獎學金

18. 共同主持的氣體水合物研究團隊研究成果榮登 Physical Chemistry Chemical Physics 期刊封面，2016

19. Editorial Board of Journal of the Taiwan Institute of Chemical Engineers (2015-2022)

20. Deputy Editor of Journal of the Taiwan Institute of Chemical Engineers (2023-now)

21. Editorial Advisory Board of ACS Journal of Chemical and Engineering Data (2021-now)

22. 論文被 Journal of Computational Chemistry 選為期刊封面(2015)

23. 王立行同學/指導教授**林祥泰**教授台灣化學工程學會 61 週年年會英語口頭報告競賽論文競賽-輸送/熱力/綠色化工/環保 C1 組佳作 (2014)

24. 趙紘毅指導教授**林祥泰**教授台灣化學工程學會 61 週年年會英語口頭報告競賽論文競賽-輸送/熱力/綠色化工/環保 C2 組佳作 (2014)

25. 陳威霖指導教授**林祥泰**教授台灣化學工程學會 61 週年年會壁報論文競賽-熱力及界面工程組佳作 (2014)

26. 趙紘毅、駱璇同學/指導教授**林祥泰**教授 2014GIMS12 會議獲得學生海報第二名

27. American Chemical Society, associate member (2000 至今)

28. American Institute of Chemical Engineers, life member

29. 台灣化工學會終身會員

30. 台灣化學工程學會理事 (2020-2022)