

**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  
Thermodynamics  
Renewable Energy

**Projects ( started from 2013 )**

1. 快速預測含化學反應系統之相行為,  
國科會 NSC 101-2628-E-002-014-MY3  
NTD 3,701,000, 08/01/2012-07/31/2015
2. 天然氣水合物資源潛能調查:熱力學與動力學研究(2/4)-分子模擬部分,  
經濟部中央地質調查所 102-5226904000-05-03  
NTD 1,150,000, 01/01/2013-12/31/2013
3. 物理性質估計和 Aspen Plus 模擬的預測模型開發: QSPR 和 COSMO-SAC 模型, (產  
業合作)  
李長榮化學工業股份有限公司  
NTD 1,449,000, 11/01/2013-04/30/2015
4. 從分子結構快速預測流體物性,  
教育部學術研究生涯發展研究計畫-深耕型研究計畫  
NTD 1,000,000, 08/01/2013-07/31/2014

**Journal Papers**

1. L.-H. Wang and **S.-T. Lin**, "A predictive method for the solubility of drug in supercritical carbon dioxide", *J. Supercrit. Fluids*, 85 81-88, 2014.(SCI)
2. T. Merker, C.M. Hsieh, **S.T. Lin**, H. Hasse, and J. Vrabec, "Fluid Phase Coexistence for the Oxidation of CO<sub>2</sub> Expanded Cyclohexane: Experiment, Molecular Simulation and COSMO-SAC", *AIChE J.*, 59 (6): 2236-2250, 2013.(SCI, EI)
3. B.S. Lee and **S.T. Lin**, "A priori prediction of the octanol-water partition coefficient (K<sub>ow</sub>) of ionic liquids", *Fluid Phase Equilib.*, in press, 2013.(SCI, EI)
4. B.S. Lee and **S.T. Lin**, "Prediction of Phase Behaviors of Ionic Liquids over a Wide Range of Conditions", *Fluid Phase Equilib.*, 356 309-320, 2013. (SCI, EI)
5. Y.-C. Kuo, C.-C. Hsu, and **S.-T. Lin**, "Prediction of Phase Behaviors of Polymer-Solvent Mixtures from the COSMO-SAC Activity Coefficient Model", *Ind. Eng. Chem. Res.*, 52 (37): 13505-13515, 2013. (SCI, EI)
6. Y.C. Hung, C.Y. Chao, C.A. Dai, W.F. Su, and **S.T. Lin**, "Band Gap Engineering via

- Controlling Donor-Acceptor Compositions in Conjugated Copolymers”, *J. Phys. Chem. B*, 117 (2): 690-696, 2013. (SCI, EI)
7. H.-Y. Chin, B.-S. Lee, Y.-P. Chen, P.-C. Chen, **S.-T. Lin**, and L.-J. Chen, “Prediction of Phase Equilibrium of Methane Hydrates in the Presence of Ionic Liquids “, *Ind. Eng. Chem. Res.*, 52 (47): 16985-16992, 2013. (SCI, EI)
  8. H.-Y. Chin, M.-K. Hsieh, Y.-P. Chen, P.-C. Chen, **S.-T. Lin**, and L.-J. Chen, “Prediction of phase equilibrium for gas hydrate in the presence of organic inhibitors and electrolytes by using an explicit pressure-dependent Langmuir adsorption constant in the van der Waals - Platteeuw model”, *J. Chem. Therm.*, 66 34-43, 2013. (SCI, EI)
  9. C.-T. Cheng, L.-J. Chen, **S.-T. Lin**, M. Tang, P.-C. Chen, and Y.-P. Chen, “Measurements for the Dissociation Conditions of Methane Hydrate in the Presence of 2,5-Dihydrofuran and 3,4-Dihydro-2H-pyran”, *Fluid Phase Equilib.*, 338 (25): 114-118, 2013. (SCI, EI)
  10. W.-L. Chen, C.-C. Hsu, and **S.-T. Lin**, “Prediction of phase behaviors of acetic acid containing fluids”, *Fluid Phase Equilib.*, 353 61-68, 2013. (SCI, EI)
  11. Y.-T. Tung, L.-J. Chen, Y.-P. Chen, and **S.-T. Lin**, “Molecular Dynamics Study on the Growth of Structure I Methane Hydrate in Aqueous Solution of Sodium Chloride”, *J. Phys. Chem. B*, 116 (48): 14115-14125, 2012.
  12. T.A. Pascal, **S.T. Lin**, W.A. Goddard, and Y. Jung, “Stability of Positively Charged Solutes in Water: A Transition from Hydrophobic to Hydrophilic”, *J. Phys. Chem. Lett.*, 3 (3): 294-298, 2012.
  13. B.S. Lee and **S.T. Lin**, “The role of long-range interactions in the phase behavior of ionic liquids”, *Phys. Chem. Chem. Phys.*, 14 (18): 6520-6525, 2012.
  14. P.-K. Lai, C.-M. Hsieh, and **S.-T. Lin**, “Rapid determination of entropy and free energy of mixtures from molecular dynamics simulations with the two-phase thermodynamic model”, *Phys. Chem. Chem. Phys.*, 14 (43): 15206-15213, 2012.
  15. M.K. Hsieh, Y.T. Yeh, Y.P. Chen, P.C. Chen, **S.T. Lin**, and L.J. Chen, “Predictive Method for the Change in Equilibrium Conditions of Gas Hydrates with Addition of Inhibitors and Electrolytes”, *Ind. Eng. Chem. Res.*, 51 (5): 2456-2469, 2012.
  16. M.K. Hsieh, W.Y. Ting, Y.P. Chen, P.C. Chen, **S.T. Lin**, and L.J. Chen, “Explicit pressure dependence of the Langmuir adsorption constant in the van der Waals-Platteeuw model for the equilibrium conditions of clathrate hydrates”, *Fluid Phase Equilib.*, 325 (15): 80-89, 2012.
  17. M.K. Hsieh and **S.T. Lin**, “Effect of mixing rule boundary conditions on high pressure (liquid plus liquid) equilibrium prediction”, *J. Chem. Therm.*, 47 33-41, 2012.
  18. C.M. Hsieh and **S.T. Lin**, “First-principles prediction of phase equilibria using the PR plus COSMOSAC equation of state”, *Asia-Pac. J. Chem. Eng.*, 7 S1-S10, 2012.
  19. H.C. Chen, C.W. Huang, J.C.S. Wu, and **S.T. Lin**, “Theoretical Investigation of the Metal-Doped SrTiO<sub>3</sub> Photocatalysts for Water Splitting”, *J. Phys. Chem. C*, 116 (14): 7897-7903, 2012.
  20. C.Y. Chao, C.H. Chao, L.P. Chen, Y.C. Hung, **S.T. Lin**, W.F. Su, and C.F. Lin, “Band

- structure engineering for low band gap polymers containing thienopyrazine”, *J. Mater. Chem.*, 22 (15): 7331-7341, 2012.
21. Y.-T. Tung, L.-J. Chen, Y.-P. Chen, and **S.-T. Lin**, “In Situ Methane Recovery and Carbon Dioxide Sequestration in Methane Hydrates: A Molecular Dynamics Simulation Study”, *J. Phys. Chem. B*, 115 (51): 15295-15302, 2011.
  22. Y.T. Tung, L.J. Chen, Y.P. Chen, and **S.T. Lin**, “Growth of Structure I Carbon Dioxide Hydrate from Molecular Dynamics Simulations”, *J. Phys. Chem. C*, 115 (15): 7504-7515, 2011.
  23. Y.S. Tai, M.T. Hsieh, M.T. Lee, D.S.H. Wong, and **S.T. Lin**, “A priori predictions of critical loci from the combined use of PRSV equation of state and the COSMO-SAC model through the MHV1 mixing rule”, *Fluid Phase Equilib.*, 308 (1-2): 25-34, 2011.
  24. A.K. Sum, **S.-T. Lin**, and J.M. Prausnitz, “A Special Tribute to Stan Sandler: The Reach and Impact of a Life-Long Dedication to the Chemical Engineering Profession”, *Ind. Eng. Chem. Res.*, 50 (1): 1-2, 2011.
  25. C.C. Shu and **S.T. Lin**, “Prediction of Drug Solubility in Mixed Solvent Systems Using the COSMO-SAC Activity Coefficient Model”, *Ind. Eng. Chem. Res.*, 50 (1): 142-147, 2011.
  26. T.A. Pascal, **S.T. Lin**, and W.A. Goddard, “Thermodynamics of liquids: standard molar entropies and heat capacities of common solvents from 2PT molecular dynamics”, *Phys. Chem. Chem. Phys.*, 13 (1): 169-181, 2011.
  27. **S.-T. Lin**, L.-H. Wang, W.-L. Chen, P.-K. Lai, and C.-M. Hsieh, “Prediction of miscibility gaps in water/ether mixtures using COSMO-SAC model”, *Fluid Phase Equilib.*, 310 (1-2): 19-24, 2011.
  28. **S.T. Lin**, “Marching into molecular design”, *Asia-Pac. J. Chem. Eng.*, 6 (2): 195-198, 2011.
  29. W.Y. Lee, T. Kurosawa, **S.T. Lin**, T. Higashihara, M. Ueda, and W.C. Chen, “New Donor-Acceptor Oligoimides for High-Performance Nonvolatile Memory Devices”, *Chem. Mater.*, 23 (20): 4487-4497, 2011.
  30. H. Kumar, B. Mukherjee, **S.T. Lin**, C. Dasgupta, A.K. Sood, and P.K. Maiti, “Thermodynamics of water entry in hydrophobic channels of carbon nanotubes”, *J. Chem. Phys.*, 134 (12): 124105, 2011.
  31. W.Y. Ko, L.J. Chen, **S.T. Lin**, and Y.P. Chen, “Measurements for the Dissociation Conditions of Methane Hydrate in the Presence of 1,3,5-Trioxane and Oxolan-2-ylmethanol”, *J. Chem. Eng. Data*, 56 (8): 3406-3410, 2011.
  32. Y.-C. Huang, J.-H. Hsu, Y.-C. Liao, W.-C. Yen, S.-S. Li, **S.-T. Lin**, C.-W. Chen, and W.-F. Su, “Employing an amphiphilic interfacial modifier to enhance the performance of a poly(3-hexyl thiophene)/TiO<sub>2</sub> hybrid solar cell”, *J. Mater. Chem.*, 21 4450- 4456, 2011.
  33. S.-N. Huang, T.A. Pascal, W.A. Goddard, P.K. Maiti, and **S.-T. Lin**, “Absolute Entropy and Energy of Carbon Dioxide Using the Two-Phase Thermodynamic Model”, *J. Chem. Theory Comput.*, 7 (6): 1893–1901, 2011.

34. M.T. Hsieh and **S.T. Lin**, "A Predictive Model for the Excess Gibbs Free Energy of Fully Dissociated Electrolyte Solutions", *AIChE J.*, 57 (4): 1061-1074, 2011.
35. C.M. Hsieh, S. Wang, **S.T. Lin**, and S.I. Sandler, "A Predictive Model for the Solubility and Octanol-Water Partition Coefficient of Pharmaceuticals", *J. Chem. Eng. Data*, 56 (4): 936-945, 2011.
36. C.M. Hsieh and **S.T. Lin**, "First-Principles Prediction of Vapor-Liquid-Liquid Equilibrium from the PR plus COSMOSAC Equation of State", *Ind. Eng. Chem. Res.*, 50 (3): 1496-1503, 2011.
37. Y.T. Tung, L.J. Chen, Y.P. Chen, and **S.T. Lin**, "The Growth of Structure I Methane Hydrate from Molecular Dynamics Simulations", *J. Phys. Chem. B*, 114 (33): 10804-10813, 2010.
38. **S.T. Lin**, P.K. Maiti, and W.A. Goddard, "Two-Phase Thermodynamic Model for Efficient and Accurate Absolute Entropy of Water from Molecular Dynamics Simulations", *J. Phys. Chem. B*, 114 (24): 8191-8198, 2010.
39. P.C. Kuo, L.J. Chen, **S.T. Lin**, and Y.P. Chen, "Measurements for the Dissociation Conditions of Methane Hydrate in the Presence of 2-Methyl-2-propanol", *J. Chem. Eng. Data*, 55 (11): 5036-5039, 2010.
40. C.M. Hsieh, S.I. Sandler, and **S.T. Lin**, "Improvements of COSMO-SAC for vapor-liquid and liquid-liquid equilibrium predictions", *Fluid Phase Equilib.*, 297 (1): 90-97, 2010.
41. C.M. Hsieh and **S.T. Lin**, "Prediction of liquid-liquid equilibrium from the Peng-Robinson plus COSMOSAC equation of state", *Chem. Eng. Sci.*, 65 (6): 1955-1963, 2010.
42. A. Debnath, B. Mukherjee, K.G. Ayappa, P.K. Maiti, and **S.T. Lin**, "Entropy and dynamics of water in hydration layers of a bilayer", *J. Chem. Phys.*, 133 (17): 174704, 2010.
43. W.-C. Yen, B. Pal, J.-S. Yang, Y.-C. Hung, **S.-T. Lin**, C.-Y. Chao, and W.-F. Su, "Synthesis and Characterization of Low Bandgap Copolymers Based on Indenofluorene and Thiophene Derivative", *J. Polym. Sci., Part A: Polym. Chem.*, 47 (19): 5044 - 5056, 2009.
44. S. Wang, **S.T. Lin**, S. Watanasiri, and C.C. Chen, "Use of GAMESS/COSMO program in support of COSMO-SAC model applications in phase equilibrium prediction calculations", *Fluid Phase Equilib.*, 276 (1): 37-45, 2009.
45. **S.-T. Lin**, M.-K. Hsieh, C.-M. Hsieh, C.-C. Hsu, and S.-N. Huang, "Reply to "Comment on "Towards the development of theoretically correct liquid activity coefficient models""", *J. Chem. Therm.*, 41 (11): 1314-1316, 2009.
46. **S.T. Lin**, M.K. Hsieh, C.M. Hsieh, and C.C. Hsu, "Towards the development of theoretically correct liquid activity coefficient models", *J. Chem. Therm.*, 41 (10): 1145-1153, 2009.
47. Y.C. Hung, J.C. Jiang, C.Y. Chao, W.F. Su, and **S.T. Lin**, "Theoretical Study on the Correlation between Band Gap, Bandwidth, and Oscillator Strength in Fluorene-Based Donor-Acceptor Conjugated Copolymers", *J. Phys. Chem. B*, 113 (24): 8268-8277,

2009.

48. M.K. Hsieh and **S.T. Lin**, “Early structural development in melt-quenched polymer PTT from atomistic molecular dynamic simulations”, *J. Phys.-Condes. Matter*, 21 (50): 505101, 2009.
49. C.M. Hsieh and **S.T. Lin**, “Prediction of 1-octanol-water partition coefficient and infinite dilution activity coefficient in water from the PR + COSMOSAC model”, *Fluid Phase Equilib.*, 285 (1-2): 8-14, 2009.
50. C.M. Hsieh and **S.T. Lin**, “First-Principles Predictions of Vapor-Liquid Equilibria for Pure and Mixture Fluids from the Combined Use of Cubic Equations of State and Solvation Calculations”, *Ind. Eng. Chem. Res.*, 48 (6): 3197-3205, 2009.

### Conference Papers

1. J.-Y. Wu and **S.-T. Lin**, “Growth of Tetrahydrofuran (THF) Clathrate Hydrates: A Molecular Dynamics Study”, 台灣化學工程學會第 60 屆年會, November 22-23, 2013. 台灣科技大學.
2. L.-H. Wang and **S.-T. Lin**, “Prediction of Drug Solubility in Supercritical Carbon Dioxide”, 台灣化學工程學會第 60 屆年會, November 22-23, 2013. 台灣科技大學.
3. H.-H. Ma and **S.-T. Lin**, “Primary Nucleation of Methane Hydrates via Molecular Dynamics Simulation”, 台灣化學工程學會第 60 屆年會, November 22-23, 2013. 台灣科技大學.
4. Y.-H. Li and **S.-T. Lin**, “Theoretical Study on the Surface Modified TiO<sub>2</sub>:P3HT Hybrid Solar Cells”, 台灣化學工程學會第 60 屆年會, November 22-23, 2013. 台灣科技大學.
5. W.-L. Chen and **S.-T. Lin**, “Simultaneous Modeling of the Vapor-Liquid and Liquid-Liquid Equilibria of Fluids Containing Acetic Acid”, 台灣化學工程學會第 60 屆年會, November 22-23, 2013. 台灣科技大學.
6. J.-Y. Wu and **S.-T. Lin**, “Growth of Tetrahydrofuran (THF) Clathrate Hydrates: A Molecular Dynamics Study”, 中華民國界面科學學會年會, July 12, 2013. 台灣大學.
7. J.-Y. Wu and **S.-T. Lin**, “Growth of Tetrahydrofuran (THF) Clathrate Hydrates: A Molecular Dynamics Study”, AIChE annual meeting, Nov. 3-8, 2013. San Francisco.
8. L.-H. Wang and **S.-T. Lin**, “Prediction of the drug solubility in Supercritical Carbon Dioxide”, SuperGreen 2013, Oct. 11-15, 2013. 義守大學.
9. L.-H. Wang and **S.-T. Lin**, “A Predictive Model to the Drug Solubility in Supercritical Carbon Dioxide”, AIChE annual meeting, Nov. 3-8, 2013. San Francisco.

10. H.-H. Ma and **S.-T. Lin**, “Primary Nucleation of Methane Hydrates via Molecular Dynamics Simulation”, The 26th International Symposium on Chemical Engineering, Dec. 6-8, 2013. Busan, Korea.
11. B.-S. Lee and **S.-T. Lin**, “Prediction of Phase Behaviors of Ionic Liquids Over a Wide Range of Conditions”, AIChE annual meeting, Nov. 3-8, 2013. San Francisco.
12. Y.-C. Hung and **S.-T. Lin**, “Band Gap Engineering on Conjugated Polymers for High Efficiency Organic Solar Cells”, Asian Consortium on Computational Materials Science, Jan 16-18, 2013. National Taiwan University of Science and Technology, Taipei, Taiwan.
13. C.-M. Hsieh, T. Merker, **S.-T. Lin**, H. Hasse, and J. Vrabec, “Application of COSMO-SAC and Molecular Simulation to An Industrially Important Pentenary System”, AIChE annual meeting, Nov. 3-8, 2013. San Francisco.
14. C.-M. Hsieh, **S.-T. Lin**, and J. Vrabec, “Understanding the Role of Dispersive Interactions in the COSMO-SAC Model”, AIChE annual meeting, Nov. 3-8, 2013. San Francisco.
15. C.-K. Chu, H.-Y. Chin, P.-C. Chen, Y.-P. Chen, **S.-T. Lin**, and L.-J. Chen, “Effect of Chain Length of Ionic Liquid On the Formation of Methane Hydrate”, AIChE annual meeting, Nov. 3-8, 2013. San Francisco.
16. Y.-P. Chen, L.-J. Chen, **S.-T. Lin**, and M. Tang, “Measurements of the Dissociation Conditions of Gas Hydrates in the Presence of Hydrocarbon Additives”, AIChE annual meeting, Nov. 3-8, 2013. San Francisco.
17. W.-L. Chen, C.-C. Hsu, and **S.-T. Lin**, “Prediction of Phase Behavior of Strongly Associating Fluids By Explicit Consideration of Transitions in Local Fluid Structures”, AIChE annual meeting, Nov. 3-8, 2013. San Francisco.
18. L.-C. Chan and **S.-T. Lin**, “Theoretical Study on Resistive Memory Devices based on Polyimides”, 第六屆全球華人理論及計算化學研討會, Jun 24-28, 2013. 淡江大學.
19. J.-Y. Wu and **S.-T. Lin**, “The Thermodynamic Stability of Tetrahydrofuran (THF) and Methane-THF Mixed Clathrate Hydrates from Molecular Dynamic Simulations”, 台灣化學工程學會第 59 屆年會, November 23-24, 2012 逢甲大學.
20. L.-H. Wang and **S.-T. Lin**, “Prediction of Drug Solubility in Supercritical Carbon Dioxide”, 台灣化學工程學會第 59 屆年會, November 23-24, 2012 逢甲大學.
21. S.-T. Lin, “Obtaining Thermodynamic Phase Diagrams in a Split Second and Prior to Experiments”, 台灣化學工程學會第 59 屆年會, November 23-24, 2012 逢甲大學.
22. P.-K. Lai and **S.-T. Lin**, “Rapid Determination of Entropy and Free Energy of Mixtures from Molecular Dynamic Simulations with the Two-Phase Thermodynamic Model”, 台灣化學工程學會第 59 屆年會, November 23-24, 2012 逢甲大學.
23. W.-L. Chen and **S.-T. Lin**, “Simultaneous Modeling of the Vapor-liquid and Liquid-Liquid Equilibria of Fluids Containing Acetic Acid”, 台灣化學工程學會第 59

屆年會, November 23-24, 2012 逢甲大學.

24. 吳軍毅, 王育倫, and 林祥泰, “以分子模擬研究甲烷水合物之融解熱在不同溫度、壓力、填滿率下的變化”, 2012 年京台兩地“化工 - 環境 - 能源”學術研討會, Aug. 21- Aug. 28, 2012. 北京化工大學.
25. L.-H. Wang and **S.-T. Lin**, “Prediction of Drug Solubility in Supercritical Carbon Dioxide Using PR+COSMOSAC Equation of State”, 2012 年京台兩地“化工 - 環境 - 能源”學術研討會, Aug. 21- Aug. 28, 2012. 北京化工大學.
26. Y.-S. Tang, Y.-H. Li, and **S.-T. Lin**, “Theoretical Study on the Surface Modified TiO<sub>2</sub>:P3HT Hybrid Solar Cells”, 2012 GSAS, Sep. 18- Sep. 21, 2012. Taipei, Taiwan.
27. T. Merker, C.-M. Hsieh, **S.-T. Lin**, H. Hasse, and J. Vrabec, “Investigation of Fluid Phase Equilibria for the Oxidation of Cyclohexane in CO<sub>2</sub> Expanded Liquids from Experiments, Molecular Simulation, PR EOS and COSMO-SAC”, Thermodynamik-Kolloquium 2012, Oct. 8- Oct. 10, 2012. Potsdam, Germany.
28. **S.-T. Lin**, “Unveiling Thermodynamic Driving Forces at the Nanoscale”, APCChE 2012, Feb. 21- Feb. 23, 2012. Singapore.
29. P.-K. Lai and **S.-T. Lin**, “Two-Phase Thermodynamic Model for Efficient and Accurate Absolute Entropy of Water From Molecular Dynamics Simulations”, AIChE 2012, Oct. 29- Nov. 2, 2012. Pittsburgh, USA.
30. P.-K. Lai and **S.-T. Lin**, “Rapid Determination of Entropy and Free Energy of Mixtures From Molecular Dynamics Simulations with the Two-Phase Thermodynamic Model”, AIChE 2012, Oct. 29- Nov. 2, 2012. Pittsburgh, USA.
31. Y.-C. Hung and **S.-T. Lin**, “Band Gap Engineering on Conjugated Polymers for High Efficiency Organic Solar Cells”, The 4th AEARUEEW 2012, Mar. 28- Mar. 30, 2012. Taipei, Taiwan.
32. C.-C. Hsu and **S.-T. Lin**, “Explicit Inclusion of Molecular Conformations in Phase Equilibrium Prediction from the PR+COSMOSAC Equation of State”, APCChE 2012, Feb. 21- Feb. 23, 2012. Singapore.
33. C.-C. Hsu, W.-L. Chen, and **S.-T. Lin**, “Prediction of Phase Behaviors of Strong Association Systems by PR+Cosmosac Equation of State”, AIChE 2012, Oct. 29- Nov. 2, 2012. Pittsburgh, USA.
34. M.-K. Hsieh, Y.-T. Yeh, W.-Y. Ting, H.-Y. Chin, P.-C. Chen, Y.-P. Chen, **S.-T. Lin**, and L.-J. Chen, “A New Thermodynamic Model for Phase Boundary of Gas Hydrates with and without Additives”, AIChE 2012, Oct. 29- Nov. 2, 2012. Pittsburgh, USA.
35. C.-M. Hsieh and **S.-T. Lin**, “Comparison of Vapor-Liquid and Liquid-Liquid Equilibrium Prediction From Combination of PRSV and COSMO-SAC Through Different Mixing Rules”, AIChE 2012, Oct. 29- Nov. 2, 2012. Pittsburgh, USA.
36. W.-L. Chen and **S.-T. Lin**, “Predicting Phase Equilibria of Strongly Associating Systems”, 2012 年京台兩地“化工 - 環境 - 能源”學術研討會, Aug. 21- Aug. 28,

2012. 北京化工大學.

37. P.Y. Tsai, Y.T. Tung, W.H. Fu, and **S.T. Lin**, "The Growth of Structure I and Structure II Methane Hydrates in the Presence of Promoters: A Molecular Dynamic Study", 台灣化學工程學會第 58 屆年會, November 25-26, 2011 成功大學.
38. Y.T. Yeh, C.H. Lin, M.K. Hsieh, **S.T. Lin**, and L.J. Chen, "Prediction of gas hydrate phase behavior in the presence of alcohols and glycols with PRSV equation of state and the vdW-P model", 7th International Conference of Gas Hydrate, July 17-21, 2011. Edinburgh, UK.
39. Y.T. Tung and **S.T. Lin**, "Growth of Methane and Carbon Dioxide Hydrates: Similarity and Differences from Molecular Dynamic Simulations", Gas Hydrate Symposium, 241st ACS National Meeting & Exposition, March 27-31, 2011. Anaheim, California, USA.
40. Y.T. Tung, L.J. Chen, and **S.T. Lin**, "Methane Hydrate Growth and its Recovery with Carbon Dioxide via Molecular Dynamics Simulations", the 7th International Conference of Gas Hydrate, July 17-21, 2011. Edinburgh, UK.
41. P.Y. Tsai, Y.T. Tung, and **S.T. Lin**, "Stability of Carbon Dioxide in Structure I and II Hydrates: A Molecular Dynamics Study", Workshop on Exploring the Structures and Dynamics of Water at Interfaces, July 15-16, 2011. National Cheng Kung University, Tainan, Taiwan.
42. P.Y. Tsai and **S.T. Lin**, "Stability of Carbon Dioxide in Structure I and II Hydrates :A Molecular Dynamics Study", The Asia Oceania Geosciences Society meeting, Aug 8-12, 2011. Taipei, Taiwan.
43. Y.S. Tang and **S.T. Lin**, "Theoretical Modeling the Performance of Bulk Heterojunction Solar Cells", 台灣化學工程學會第 58 屆年會, November 25-26, 2011. 成功大學.
44. **S.T. Lin**, "Dominating factors for the Growth of Clathrate Hydrates: A Molecular Dynamics Simulation Study", the Workshop on Dynamics and Structure of Water: From Gas Phase Clusters to Condensed Phase, Oct 15-16, 2011. Taipei, Taiwan.
45. Y.C. Hung and **S.T. Lin**, "Theoretical investigation on electron transfer between packed PCBM and ThCBM", 台灣化學工程學會第 58 屆年會, November 25-26, 2011. 成功大學.
46. C.C. Hsu and **S.T. Lin**, "Prediction of Conformation Distribution Under Various Solvent", 台灣化學工程學會第 58 屆年會, November 25-26, 2011. 成功大學.
47. C.C. Hsu and **S.T. Lin**, "Prediction of Conformation Distribution with the PR+COSMOSAC Equation of State", AIChE Annual Meeting, Oct 16-21, 2011. Minneapolis, Minnesota, USA.
48. M.K. Hsieh, Y.T. Yeh, Y.P. Chen, **S.T. Lin**, and L.J. Chen, "Electrolyte Effect on the Phase Behavior of Gas Hydrates Predicted by Using Fugacity-Based Model Composed of PRSV EoS, COSMO-SAC Liquid Model, and vdW-P Model", The Asia Oceania Geosciences Society meeting, Aug 8-12, 2011. Taipei, Taiwan.



49. W.H. Fu, Y.T. Tung, and **S.T. Lin**, “The Growth of Structure II Methane Hydrates with Promoters by Molecular Dynamics Simulations”, Workshop on Exploring the Structures and Dynamics of Water at Interfaces, July 15-16, 2011. National Cheng Kung University, Tainan, Taiwan.
50. C.T. Cheng, L.J. Chen, **S.T. Lin**, M. Tang, and Y.P. Chen, “Measurement for the Dissociation Conditions of Methane Hydrates in the Presence of Additives”, The 7th International Conference of Gas Hydrate, July 17-21, 2011. Edinburgh, UK.
51. L.C. Chan and **S.T. Lin**, “DFT Study on the Switching Mechanism of Polymer Memory Devices”, 台灣化學工程學會第 58 屆年會, November 25-26, 2011. 成功大學.
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53. Y.T. Tung and **S.T. Lin**, “Molecular dynamics simulation study on the growth mechanism of carbon dioxide hydrate”, APCChE 2010, October 5-8, 2010. Taipei, Taiwan.
54. K.Y. Tseng and **S.T. Lin**, “Molecular dynamics simulation study on electrical double layer nano-capacitors”, APCChE 2010, October 5-8, 2010. Taipei, Taiwan.
55. **S.T. Lin**, L.H. Wang, W.L. Chen, P.K. Lai, and C.M. Hsieh, “Prediction of Miscibility Gaps in Water/Ether Mixtures Using COSMO-SAC Model”, AIChE Annual Meeting, November 7-12, 2010. Salt Lake City, Utah, USA.
56. **S.T. Lin**, “A Priori Phase Equilibria Predictions from First-Principles Solvation Calculations”, AIChE Annual Meeting, November 7-12, 2010. Salt Lake City, Utah, USA.
57. Y.C. Hung and **S.T. Lin**, “Theoretical study on stacking effects of optical and electronic properties of conjugated polymer”, APCChE 2010, October 5-8, 2010. Taipei, Taiwan.
58. S.N. Hung and **S.T. Lin**, “Absolute Entropy and Free Energy of Pure Fluids from Molecular Dynamic Simulations”, APCChE 2010, October 5-8, 2010. Taipei, Taiwan.
59. C.C. Hsu and **S.T. Lin**, “Prediction of Octanol-water Partition Coefficient of Ionic Liquids”, APCChE 2010, October 5-8, 2010. Taipei, Taiwan.
60. C.M. Hsieh, S.I. Sandler, and **S.T. Lin**, “Revision and Extension of the COSMO-SAC Model”, AIChE Annual Meeting, November 7-12, 2010. Salt Lake City, Utah, USA.
61. C.M. Hsieh and **S.T. Lin**, “First-principles prediction of phase equilibrium”, APCChE 2010, October 5-8, 2010. Taipei, Taiwan.
62. C.M. Hsieh and **S.T. Lin**, “Prediction of VLE, LLE, and VLLE using the Peng-Robinson+COSMOSAC equation of state”, PPEPPD 2010, May 16-21, 2010. Suzho, China.
63. H.C. Chen and **S.T. Lin**, “Theoretical Investigation of Charge Transfer in Conjugated Polymers”, APCChE 2010, October 5-8, 2010. Taipei, Taiwan.

64. N.Y. Chang and **S.T. Lin**, "An Optoelectrical Model for Organic Bulk Heterojunction Solar Cells", APCCChE 2010, October 5-8, 2010. Taipei, Taiwan.
65. M.K. Hsieh and **S.T. Lin**, "Isothermal Crystallization in the Nematic Phase of Poly(Trimethylene Terephthalate) Fibers by Molecular Dynamic Simulations", AIChE Annual Meeting, November 8-13, 2009 Nashville, TN, USA.
66. Y.T. Tung and **S.T. Lin**, "Study of the Growth Mechanism of Methane Hydrate by MD Simulations", 台灣化學工程學會第 56 屆年會, November 27-28, 2009. 中興大學.
67. Y.T. Tung and **S.T. Lin**, "A Study of the Growth Mechanism of Methane Hydrate using MD Simulations" AOGS2009 Annual Meeting", AOGS2009 Annual Meeting, Aug 11-15, 2009. Singapore.
68. P.Y. Tsai and **S.T. Lin**, "A Theoretical model for Conjugated Polymer Solar Cells", 台灣化學工程學會第 56 屆年會, November 27-28, 2009. 中興大學.
69. **S.T. Lin**, Y.P. Chen, and L.J. Chen, "Thermodynamics Study of Gas Hydrates: Experiment, Modeling, and Molecular Simulation", Taiwan-Germany joint Symposium on marine gas hydrate exploration and carbon sequestration technologies, November 4-5, 2009. Beijing, China.
70. **S.T. Lin**, "Theoretical Modeling of Bulk Heterojunction Solar Cells: A Chemical Engineer's Perspective", 台灣化學工程學會第 56 屆年會, November 27-28, 2009. 中興大學.
71. **S.T. Lin**, "A Predictive Model for the Thermodynamic Properties of Electrolyte Solutions", The 5th Sino-US Conference of Chemical Engineering, October 13-16, 2009. Beijing, China.
72. **S.T. Lin**, "Prediction of Thermodynamic Properties of Fluids from Molecular Structures", The 2009 Workshop on Nanotechnology and Solar Cells, and Green Chemical Processes and Materials, March 7-8, 2009. Ming Chi University of Technology, Taiwan.
73. Y.C. Hung and **S.T. Lin**, "Theoretical Study On Electronic And Optical Properties Of Conjugated Polymers", The fourth Asian Pacific Conference on Theoretical & Computational Chemistry (APCTCC-4), December 21-23, 2009. Port Dickson, Malaysia.
74. C.C. Hsu and **S.T. Lin**, "Development of New Thermodynamic Models via Coordination Number", 台灣化學工程學會第 56 屆年會, November 27-28, 2009. 中興大學.
75. C.M. Hsieh and **S.T. Lin**, "Prediction of Vapor-Liquid and Liquid-Liquid Equilibria of Mixtures From Peng-Robinson+COSMOSAC Equation of State", AIChE Annual Meeting, November 8-13, 2009. Nashville, TN, USA.

## Book Chapter

1. **S.T. Lin** and C.M. Hsieh, Obtaining Thermodynamic Properties and Fluid Phase Equilibria without Experimental Measurements, in *Application of Thermodynamics to Biological and Materials Science*, Mizutani Tadashi (Ed). 2011, 459-482. Intech.

### Honors and Others

1. 台灣大學 101 學年度教學優良教師「教學優良獎」(2013)
2. 吳軍毅同學/指導教授**林祥泰**教授台灣化學工程學會 60 週年年會研究生英語專題報告競賽佳作, 2012/11/23-24
3. KAIST IT Convergence Campus Global Lecturer (2012/12/4-6)
4. 吳軍毅同學/指導教授**林祥泰**教授台灣化學工程學會 59 週年年會能源工程組壁報論文競賽佳作, 2012/11/23-24
5. 陳威霖同學/指導教授**林祥泰**教授台灣化學工程學會 59 週年年會熱力及界面工程組 (Thermodynamics) 壁報論文競賽佳作, 2012/11/23-24
6. 台灣化學工程學會傑出論文-化工傑作獎 (共同作者蔡佩紋同學、陳延平教授、陳立仁教授) (2012)
7. 台灣大學 100 學年度優良導師 (2012)
8. 台灣大學 100 學年度教學優良教師 (2012)
9. Editorial Board of The Scientific World Journal (2012)
10. 蔡佩紋、董彥佃、傅維萱同學/指導教授**林祥泰**教授台灣化學工程學會 58 週年年會熱力及界面工程組 (Thermodynamics) 壁報論文競賽佳作, 2011/11/25-26
11. 第二屆財團法人李謀偉福聚教育基金會傑出教授獎 (2011/8)
12. 台灣大學 99 學年度教學優良教師 (2011)
13. Editorial Board of Open Journal of Physical Chemistry (2011)
14. 第六屆國際流體性質預測競賽 (Sixth Industrial Fluid Properties Simulation Challenge) 季軍 (2010)
15. 謝介銘同學/指導教授**林祥泰**教授 第 13 屆亞太化工會議 (2010 APCCHE Congress) 大會最佳海報論文獎 (全會僅選一篇), 2010/10/05-08
16. 張乃元同學/指導教授**林祥泰**教授 第 13 屆亞太化工會議 (2010 APCCHE Congress)

計算分子科學與工程組 (Computational Molecular Science and Engineering) 最佳海報論文獎 (best poster paper award) , 2010/10/05-08

17. 謝介銘同學/指導教授林祥泰教授 第 13 屆亞太化工會議 (2010 APCCHE Congress) 熱力學組 (Thermodynamics) 最佳海報論文獎 (best poster paper award) , 2010/10/05-08
18. 國科會吳大猷先生紀念獎 , 2010/08/09
19. 台灣大學 98 學年度教學優良教師 (2010)
20. Editorial Board of Global Journal of Physical Chemistry (2010)
21. 台灣大學 97 學年度教學優良教師 (2009)
22. 第五屆國際流體性質預測競賽 (Fifth Industrial Fluid Properties Simulation Challenge) 冠軍 (2008)
23. American Chemical Society, associate member (2000 至今)
24. American Institute of Chemical Engineers, associate member (1999 至今)

