

**Li-Chiang Lin, Ph.D.**

Assistant Professor

The Umit S. Ozkan Professorship

William G. Lowrie Dept. of Chemical and Biomolecular Engineering  
CBEC514, 151 W. Woodruff Ave., Columbus, OH 43210

The Ohio State University

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Group website: <https://lin-group.engineering.osu.edu/>**EDUCATION**

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|-------------------------|--|
| 2010 Sep.-<br>2014 May  | <b>Ph.D., Chemical and Biomolecular Engineering, University of California-Berkeley, USA</b><br>Thesis: "Computational Study of Porous Materials for Gas Separations"                     |
| 2006 Feb.-<br>2007 Oct. | <b>M.S., Chemical Engineering, National Taiwan University, Taiwan</b><br>Thesis: "Effects of Relative Volatility Ranking to the Design of Reactive Distillation: Excess-reactant Design" |
| 2002 Sep.-<br>2006 Jan. | <b>B.S., Chemical Engineering, National Taiwan University, Taiwan</b>  |

**ACADEMIC APPOINTMENTS**

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|-----------------------------------|--|
| 2016 Sep.-<br>2016 Jul. -<br>Aug. | Assistant Professor, Dept. Chemical and Biomolecular Engineering, The Ohio State University                  |
| 2016 Jan.-<br>Jun.                | Visiting Assistant Professor, Dept. of Chemical and Biomolecular Engineering, The Ohio State University      |
| 2015 Jan.-<br>Nov.                | Research Scientist, Dept. of Materials Science and Engineering, MIT (Prof. Jeffrey C. Grossman's group)      |
| 2015                              | Assistant Professor, Dept. of Process and Energy, Delft University of Technology, the Netherlands            |
| 2014-2015                         | Visiting Scientist, Dept. of Materials Science and Engineering, MIT (Prof. Jeffrey C. Grossman's group)      |
| 2014                              | Postdoctoral Researcher, Dept. of Materials Science and Engineering, MIT (Prof. Jeffrey C. Grossman's group) |
| 2011-2014                         | Junior Specialist, Dept. of Chemical and Biomolecular Engineering, UC-Berkeley (Prof. Berend Smit's group)   |
| 2009-2010                         | Graduate Student Researcher, UC-Berkeley and Lawrence Berkeley National Lab                                  |
|                                   | Teaching Assistant, Dept. of Chemical Engineering, National Taiwan University, Taiwan                        |

**NON-ACADEMIC APPOINTMENTS**

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| 2008-2009 | Integrating Process Engineer, Taiwan Semiconductor Manufacturing Corporation (TSMC) |
| 2007-2008 | Corporal, Army, Taiwan (Mandatory military service)                                 |

**SELECTED HONORS**

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| 2020 | Charles E. MacQuigg Award for Outstanding Teaching, College of Engineering, The Ohio State University, USA |
| 2020 | Lumley Research Award, College of Engineering, The Ohio State University, USA                              |
| 2019 | Excellence in Publications Award, International Adsorption Society (IAS)                                   |

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2013	DOW Excellence in Teaching Award, University of California – Berkeley, USA
2012-2013	Chevron Fellowship, USA
2012	Graduate Student Research Award, AIChE Separation Division, USA
2012-2014	Government Fellowship for Study Abroad, Ministry of Education, Taiwan
2010	Power Top-Off Award, University of California – Berkeley, USA
2005	Memorial Scholarship for Mr. Lin, Hsiung-Chen, Taiwan
2003-2005	Presidential Award, Top 5% students - ( <b>Six times</b> ), National Taiwan University, Taiwan
2003-2005	First Bank Scholarship for Outstanding College Students - ( <b>Three times</b> ), Taiwan
2004	AZ Electronic Materials Scholarship, Taiwan
2003	TASCO Chemical Corporation Scholarship, Taiwan

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**PUBLICATIONS (67 published articles; h-index 29 and total citations ~3400)**

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Google Scholar profile (<https://scholar.google.com/citations?user=9yluyaQAAAAJ&hl=en>)

**Following Appointment at The Ohio State University in Fall 2016**

67. Zou, C.; Penley, D. R.; Cho, E. H.; Lin, L.-C.\* Efficient and Accurate Charge Assignments via Multi-Layer Connectivity-based Atom Contribution (m-CBAC) Approach, *J. Phys. Chem. C*, just accepted, **2020**.
66. Risplendi, F.; Raffone, F.; Lin, L.-C.; Grossman, J.C.; Cicero, G. Fundamental Insights on Hydration Environment of Boric Acid and Its Role in Separation from Saline Water, *J. Phys. Chem. C*, 124, 1438-1445, **2020**.
65. Su, C.-Y.; Lyu, Q.; Kang, D.-Y.\*; Yang, Z.-H.; Lam, C. H.; Chen, Y.-H.; Lo, S.-C.; Hua, C.-C.\* & **Lin, L.-C.\*** Hexagonal superalignment of nano-objects with tunable separation in a dilute and spacer-free solution, *Phys. Rev. Lett.*, 123, 238002, **2019**.
64. Cho, E. H. & **Lin, L.-C.\*** Electrostatic Potential Optimized Molecular Models for Molecular Simulations: CO, CO<sub>2</sub>, COS, H<sub>2</sub>S, N<sub>2</sub>, N<sub>2</sub>O, and SO<sub>2</sub>, *J. Chem. Theory Comput.*, 15 (11), 6323-6332, **2019**.
63. Kan, M.-Y.; Shin, J. H.; Yang, C.-T.; Chang, C.-K.; Lee, L.-W.; Chen, B.-H.; Lu, K.-L.; Lee, J. S.\*; **Lin, L.-C.\*** & Kang, D.-Y.\* Activation-Controlled Structure Deformation of Pillared-Bilayer Metal-Organic Framework Membranes for Gas Separations, *Chem. Mater.*, 31 (18), 7666-7677, **2019**.
62. Sinha, P.; Datar, A.; Jeong, C.; Deng, X.; Chung, Y. G. & **Lin, L.-C.\*** Surface Area Determination of Porous Materials Using the Brunauer-Emmett-Teller (BET) Method: Limitations and Improvements, *J. Phys. Chem. C*, 123, 20195-20209, **2019**.
61. Lyu, Q.; Deng, X.; Hu, S.; **Lin, L.-C.\*** & Ho, W.S.H. Exploring the Potential of Defective UiO-66 as Reverse Osmosis Membranes for Desalination, *J. Phys. Chem. C*, 123, 16118-16126, **2019**.
60. Yu, Y.; Chien, S.-C.; Sun, J.; Hettiaratchy, E.C.; Myers, R.C.; **Lin, L.-C.\*** & Wu, Y.\* Excimer Formation and Long-Lived Charge Separation in Self-Assembled Dyes on Metal Oxides, *J. Am. Chem. Soc.*, 141, 8727-8731, **2019**.
59. Cho, E.H.; Lyu, Q. & **Lin, L.-C.\*** Computational Discovery of Nanoporous Materials for Energy- and Environment-related applications, *Mol. Sim.*, in press, **2019**.
58. Yu, Y.; Click, K. A.; Chien, S.-C.; Sun, J.; Curtze, A.; **Lin, L.-C.\*** & Wu, Y.\* Decoupling pH-Dependence of Flat-Band Potential in Aqueous Dye-Sensitized Electrodes, *J. Phys. Chem. C*, 123, 8681-8687, **2019**.
57. Mohona, T. M.; Gupta, A.; Masud, A.; Chien, S.-C.; **Lin, L.-C.**; Nalam, P. C. & Aich, N. Aggregation Behavior of Inorganic 2D Nanomaterials Beyond Graphene: Insights from Molecular Modeling and Modified DLVO Theory, *Environ. Sci. Technol.*, 53, 4161-4172, **2019**.

56. Deshpande, N.; Cho, E.H.; Spanos, A.P.; **Lin, L.-C.** & Brunelli, N.A. Tuning Molecular Structure of Tertiary Amine Catalysts for Glucose Isomerization, *J. Catal.* 372, 119-127, **2019**.
55. Janda, A.; **Lin, L.-C.**; Vlasisavljevich, B.; Van der Mynsbrugge, J.; Bell, A. T., RE: "Impact of Zeolite Structure on Entropic-Enthalpic Contributions to Alkane Monomolecular Cracking: An IR Operando Study" by S. A. Kadam, H. Li, R. F. Wormsbacher, A. Travert, *Chem. Eur. J.*, 25, 7225-7226, **2019**.
54. Cho, E.H. & **Lin, L.-C.\***, Systematic Molecular Model Development with Reliable Charge Distributions for Gaseous Adsorption in Nanoporous Materials, *J. Mater. Chem. A* 6, 16029-16042, **2018**.
53. Lim, J.R.; Yang, C.-T.; Kim, J. & **Lin, L.-C.\***, Transferability of CO<sub>2</sub> Force Fields for the Prediction of Adsorption Properties in All-Silica Zeolites, *J. Phys. Chem. C* 122, 10892-10903, **2018**.
52. Becker, T.; Luna-Triguero, A.; Vicent-Luna, J.M.; **Lin, L.-C.**; Dubbeldam, D.; Calero, S. & Vlugt, T. Potential of Polarizable Force Fields for Predicting the Separation Performance of Small Hydrocarbons in M-MOF-74, *Phys. Chem. Chem. Phys.* 20, 28848-28859, **2018**.
51. Becker, T.; **Lin, L.-C.**; Dubbeldam, D. & Vlugt, T. Polarizable Force Field for CO<sub>2</sub> in M-MOF-74 Derived from Quantum Mechanics, *J. Phys. Chem. C* 122, 24488-24498, **2018**.
50. Bien, C.E; Chen, K.K.; Chien, S.-C.; Reiner, B.R.; **Lin, L.-C.**; Wade, C.R.\* & Ho, W.S.W. A Bioinspired Metal-Organic Framework for Trace CO<sub>2</sub> Capture, *J. Am. Chem. Soc.* 140, 12662-12666, **2018**.
49. Zou, C. & **Lin, L.-C.\*** Exploring the Potential and Design of Zeolite Nanosheets as Pervaporation Membranes for Ethanol Extraction, *Chem. Commun.* 54, 13200-13203, **2018**. \*\*\* Featured as the inside front cover of the issue
48. Yang, C.-T.; Kshiragar, A.R; Charaf Eddin, A.; **Lin, L.-C.\*** & Poloni, R.\*, Tuning Gas Adsorption by Metal Node-Blocking in Photoresponsive Metal-Organic Frameworks, *Chem. Eur. J.* 24, 15167-15172, **2018**. \*\*\* Featured as the frontispiece of the issue
47. Lyu, Q.; Sun, S.; Li, C.; Hu, S. & **Lin, L.-C.\***, Rational Design of Two-dimensional Hydrocarbon Polymer as Ultrathin-film Nanoporous Membranes for Water Desalination, *ACS Appl. Mater. Interfaces* 10, 18778-18786, **2018**.
46. Chen, Y.-R.; Liou, K.-H.; Kang, D.-Y.; Chen, J.-J. & **Lin, L.-C.\***, Investigation of the Water Adsorption Properties and Structural Stability of MIL-100(Fe) with Different Anions, *Langmuir* 34, 4180-4187, **2018**.
45. Yang, C.-T.; Janda, A.; Bell, A.T.\* & **Lin, L.-C.\***, Atomistic Investigations of the Effects of Si/Al Ratio and Al Distribution on the Adsorption Selectivity of n-Alkanes in Brønsted-Acid Zeolites, *J. Phys. Chem. C* 122, 9397-9410, **2018**. \*\*\* Featured as the cover of the issue
44. Cho, J.W.; **Lin, L.-C.\***, & Grossman, J.C.\*, The Role of Structural Defects in the Water Adsorption Properties of MOF-801, *J. Phys. Chem. C* 122, 5545-5552, **2018**.
43. Van der Mynsbrugge, J.; Janda, A.; **Lin, L.-C.**; Van Speybroeck, V.; Head-Gordon, M. & Bell, A.T., Understanding Brønsted-Acid Catalyzed Monomolecular Reactions of Alkanes in Zeolite Pores by Combining Insights from Experiment and Theory, *ChemPhysChem* 19, 341-358, **2018**. \*\*\* Featured as the cover of the issue and highlighted in the cover profile.
42. Jamali, S.H.; Vlugt, T.J.H & **Lin, L.-C.\***, Atomistic Understanding of Zeolite Nanosheets for Water Desalination, *J. Phys. Chem. C* 121, 11273-11280, **2017**. \*\*\* Selected as the ACS Editors' Choice and featured as the cover of the issue
41. **Lin, L.-C.**; Paik, D. & Kim, J., Understanding Gas Adsorption in MOF-5/Graphene Oxide Composite Material, *Phys. Chem. Chem. Phys.* 19, 11639-11644, **2017**.

40. Deshpande, N.; Pattanaik, L.; Whitaker, M.W.; Yang, C.-T.; **Lin, L.-C.** & Brunelli, N.A., Selectively Converting Glucose to Fructose Using Immobilized Tertiary Amines, *J. of Catalysis* 353, 205-210, **2017**.
39. Van der Mynsbrugge, J.; Janda, A.; Mallikarjun Sharada, S.; **Lin, L.-C.**; Van Speybroeck, V.; Head-Gordon, M. & Bell, A., Theoretical Analysis of the Influence of Pore Geometry on Monomolecular Cracking and Dehydrogenation of n-Butane in Brønsted-Acid Zeolites, *ACS Catalysis* 7, 2685-2697, **2017**.
38. Liou, K.-H.; Kang, D.-Y. & **Lin, L.-C.\***, Investigating the Potential of Single-walled Aluminosilicate Nanotubes in Water Desalination, *ChemPhysChem* 18, 179-183, **2017**. \*\*\*Featured as the back cover of the issue
37. Becker, T.; Heinen, J.; Dubbeldam, D.; **Lin, L.-C.** & Vlugt, T., Polarizable Force Fields for CO<sub>2</sub> and CH<sub>4</sub> Adsorption in M-MOF-74, *J. Phys. Chem. C* 121, 4659-4673, **2017**.
36. Janda, A.; Vlaisavljevich, B.; Smit, B.; **Lin, L.-C.\*** & Bell, A.T.\*, Effects of Zeolite Pore and Cage Topology on Thermodynamics of n-Alkane Adsorption at Brønsted Protons in Zeolites at High Temperature, *J. Phys. Chem. C* 121, 1618-1638, **2017**.
35. De Lange, M.F.; **Lin, L.-C.**; Gascon, J.; Vlugt, T.J.H. & Kapteijn, F., Assessing the surface area of porous solids – limitations, probe molecules and methods, *Langmuir* 32, 12664-12675, **2016**.

### **Prior to Appointment at The Ohio State University**

34. (†Contributed equally) †Cohen-Tanugi, D.; †**Lin, L.-C.** & Grossman, J.C., Multilayer Nanoporous Graphene Membranes for Water Desalination, *Nano Lett.* 16, 1027-1033, **2016**.
33. Fan, Z.; **Lin, L.-C.**; Buijs, W.; Vlugt, T.J.H. & van Huis, M.A., Atomistic understanding of cation exchange in PbS nanocrystals using simulations with pseudoligands, *Nature Communications* 7, 11503, **2016**.
32. Braun, E.; Zurhelle, A.F.; Thijssen, W.; Kchnell, S.K.; **Lin, L.-C.**; Kim, J.; Thompson, J.A. & Smit, B., High-Throughput Computational Screening of Nanoporous Adsorbents for CO<sub>2</sub> Capture from Natural Gas, *Molecular Systems Design & Engineering* 1, 175-188 **2016**. \*\*\*Featured as the cover of the issue
31. Mercado, R.; Vlaisavljevich, B; **Lin, L.-C.**; Lee, K.; Lee, Y.; Mason, J.A.; Xiao, D.J.; Gonzalez, M.I.; Kapelewski, M.T.; Neaton, J.B. & Smit, B., Force Field Development from Periodic Density Functional Theory Calculations for Gas Separation Applications Using Metal-Organic Frameworks, *J. Phys. Chem. C* 120, 12590-12604, **2016**.
30. Janda, A.L.; Vlaisavljevich, B.; **Lin, L.-C.**; Smit, B. & Bell, A.T., Effects of zeolite structural confinement on adsorption thermodynamics and reaction kinetics for monomolecular cracking and dehydrogenation of n-butane, *J. Am. Chem. Soc.* 138, 4739-4756, **2016**.
29. Becker, T.; Dubbeldam, D.; **Lin, L.-C.** & Vlugt, T., Investigating polarization effects of CO<sub>2</sub> adsorption in MgMOF-74, *J. Comput. Sci.* 15, 86-94, **2016**.
28. **Lin, L.-C.** & Grossman, J.C., Atomistic Understandings of Reduced Graphene Oxide as an Ultrathin-Film Nanoporous Membrane for Separations, *Nature Communications* 6, 8335, **2015**.
27. **Lin, L.-C.**; Choi, J. & Grossman, J.C., Two-dimensional Covalent Triazine Framework as an Ultrathin-Film Nanoporous Membrane for Desalination, *Chem. Commun.* 51, 14921-14924, **2015**.
26. (†Contributed equally) †Lee, K.; †Howe, J.; †**Lin, L.-C.**; Smit, B. & Neaton, J.B., Small Molecule Adsorption in Open-Site Metal-Organic Frameworks: a Systematic Density Functional Theory Study for Rational Design. *Chem. Mater.* 27, 668-678, **2015**.
25. (†Contributed equally) †Peng, X.; †**Lin, L.-C.**; Sun, W. & Smit, B., Water Adsorption in Metal-Organic

- Frameworks with Open-Metal Sites. *AICHE J.* 61, 677-687, **2015**.
24. Braun, E.; Chen, J.J.; Schnell, S.K.; **Lin, L.-C.**; Reimer, J.A. & Smit, B., Nanoporous Materials can Tune the Critical Point of a Pure Substance, *Angew. Chem. Int. Ed.* 54, 14349-14352, **2015**.
23. De Lange, M.; Van Velzen, B.; Ottevanger, C.; Verouden, K.; **Lin, L.-C.**; Vlugt, T.; Gascon, J. & Kateijn, F., Metal-Organic Frameworks in Adsorption Driven Heat Pumps: The Potential of Alcohols as Working Fluid, *Langmuir* 31, 12783-12796, **2015**.
22. Janda, A.L.; Vlaisavljevich, B.; **Lin, L.-C.**; Sharada, S.M.; Smit, B.; Head-Gordon, M. & Bell, A.T., Adsorption Thermodynamics and Intrinsic Activation Parameters for Monomolecular Cracking of N-alkanes on Brønsted-acid Sites in Zeolites, *J. Phys. Chem. C.* 119, 10427-10438, **2015**.
21. (†Contributed equally) †Liu, H.; †Liu, B.; †**Lin, L.-C.**; Chen, G.-J.; Wu, Y.-Q.; Wang, J.; Gao, X.-T.; Lv, Y.-L.; Pan, Y.; Zhang, X.-X.; Zhang, X.-R.; Yang, L.-Y.; Sun, C.-Y.; Smit, B. & Wang, W.-C., A Hybrid Absorbent-Adsorbent Method to Efficiently Capture Carbon. *Nature Communications* 5, 5147, **2014**.
20. **Lin, L.-C.**; Lee, K.; Gagliardi, L.; Neaton, J.B. & Smit, B., Force Field Development from Electronic Structure Calculations with Periodic Boundary Conditions: Applications to Gaseous Adsorption and Transport in Metal-Organic Frameworks. *J. Chem. Theory Comput.* 10, 1477-1488, **2014**.
19. (†Contributed equally) †Borycz, J.; †**Lin, L.-C.**; Bloch, E.D.; Kim, J.; Dzubak, A.L.; Maurice, R.; Semrouni, D.; Lee, K.; Smit, B. & Gagliardi, L., CO<sub>2</sub> Adsorption in Fe<sub>2</sub>(dobdc): A Classical Force Field Parameterized from Quantum Mechanical Calculations, *J. Phys. Chem. C* 118, 12230-12240, **2014**.
18. Huck, J.M.; **Lin, L.-C.**; Berger, A.; Shahrak, M.N.; Martin, R.L.; Bhowm, A.S.; Haranczyk, M.; Reuter, K. & Smit, B., Evaluating different classes of porous materials for carbon capture, *Energy Environ. Sci.* 7, 4132-4146, **2014**.
17. Sun, W.; **Lin, L.-C.**; Peng, X. & Smit, B., Screening of Porous MOFs and Zeolites for the Removal of SO<sub>2</sub> and NO<sub>x</sub> in the Flue Gases: a Molecular Simulation Study. *AICHE J.* 60, 2314-2323, **2014**.
16. Simon, C.; Kim, J.; **Lin, L.-C.**; Martin, R.L.; Haranczyk, M. & Smit, B., Optimizing Nanoporous Materials for Gas Storage, *Phys. Chem. Chem. Phys.* 16, 5499-5513, **2014**. \*\*\*Featured as the cover of the issue
15. Lee, J.; Isley, W.C.; Dzubak, A.L.; Verma, P.; Stoneburner, S.J.; **Lin, L.-C.**; Howe, H.D.; Bloch, E.D.; Reed, D.A.; Hudson, M.R.; Brown, C.M.; Long, J.R.; Neaton, J.B.; Smit, B.; Cramer, C.H.; Truhlar, D.G. & Gagliardi, L., Design of a Metal-Organic Framework with Enhanced Back Bonding for the Separation of N<sub>2</sub> and CH<sub>4</sub>, *J. Am. Chem. Soc.* 136, 698-704, **2014**.
14. Kim, J.; **Lin, L.-C.**; Lee, K.; Neaton, J.B. & Smit, B., Efficient Determination of Accurate Force Fields for Porous Materials Using Ab-initio Total Energy Calculations, *J. Phys. Chem. C* 118, 2693-2701, **2014**.
13. Bloch, E.D.; Hudson, M.R.; Mason, J.A.; Chavan, S.; Crocella, V.; Howe, J.D.; Lee, K.; Dzubak, A.L.; Queen, W.K.; Zadrozny, J.M.; Geier, S.J.; **Lin, L.-C.**; Gagliardi, L.; Smit, B.; Neaton, J.B.; Brodiga, S.; Brown, C.M. & Long, J.R., Reversible CO Binding Enables Tunable CO/H<sub>2</sub> and CO/N<sub>2</sub> Separations in Metal-Organic Frameworks with Exposed Divalent Metal Cations, *J. Am. Chem. Soc.* 136, 10752-10761, **2014**.
12. **Lin, L.-C.**; Kim, J.; Kong, X.; Scott, E.; McDonald, T.M.; Long, J.R.; Reimer, J.A. & Smit, B., Understanding CO<sub>2</sub> Dynamics in Metal-Organic Frameworks with Open Metal Sites, *Angew. Chem. Int. Ed.* 52, 4410-4413, **2013**. \*\*\*Featured as the inside cover of the issue
11. Kim, J.; Abouelnasr, M.; **Lin, L.-C.** & Smit, B., Large-scale Screening of Zeolite Structures for CO<sub>2</sub> Membrane Separation, *J. Am. Chem. Soc.* 135, 7545-7552, **2013**.
10. Swisher, J.A.; **Lin, L.-C.**; Kim, J. & Smit, B., Evaluating Mixture Adsorption Models Using Molecular

- Simulation, *AICHE J.* 59, 3054-3064, **2013**.
9. Haranczyk, M.; **Lin, L.-C.**; Lee, K.; Neaton, H.B. & Smit, B., Methane Storage Capabilities of Diamond Analogues, *Phys. Chem. Chem. Phys.* 15, 20937-20942, **2013**.
  8. Martin, R.L.; **Lin, L.-C.**; Jariwala, K.; Smit, B. & Haranczyk, M., Mail-Order Organic Frameworks (MOFs): Designing Isorecticular MOF-5 Analogues Comprising Commercially Available Organic Molecules, *J. Phys. Chem. C* 117, 12159-12167, **2013**. \*\*\*Featured as the cover of the issue
  7. Planas, N.; Dzubak, A.L.; Poloni, R.; **Lin, L.-C.**; McManus, A.; McDonald, T.M.; Neaton, J.B.; Long, J.R.; Smit, B. & Gagliardi, L., The Mechanism of Carbon Dioxide Adsorption in an Alkylamine-Functionalized Metal-Organic Framework, *J. Am. Chem. Soc.* 135, 7402-7405, **2013**.
  6. Kim, J.; Maiti, A.; **Lin, L.-C.**; Stolaroff, J.K.; Smit, B. & Aines, R.D., New Materials for Methane Capture from Dilute and Medium-concentration Sources,” *Nature Communications* 4, 1694, **2013**.
  5. (†Contributed equally) †Kim, J.; †**Lin, L.-C.**; Swisher, J.A.; Haranczyk, M. & Smit, B. Prediction Large CO<sub>2</sub> Adsorption in Aluminosilicate Zeolites for Postcombustion Carbon Dioxide Capture, *J. Am. Chem. Soc.* 134, 18940-18943, **2012**.
  4. **Lin, L.-C.**; Berger, A.H.; Martin, R.L.; Kim, J.; Swisher, J.A.; Jariwala, K.; Rycroft, C.H.; Bhowm, A.S.; Deem, M.W.; Haranczyk, M. & Smit, B., In Silico Screening of Carbon-Capture Materials, *Nature Materials* 11, 633-641, **2012**.
  3. (†Contributed equally) †Kim, J.; †**Lin, L.-C.**; Martin, R.L.; Swisher, J.A.; Haranczyk, M. & Smit, B., Large-scale Computational Screening of Zeolites for Ethane/Ethene Separation, *Langmuir* 28, 11914-11919, **2012**.
  2. (†Contributed equally) †Dzubak, A.L.; †**Lin, L.-C.**; Kim, J.; Swisher, J.A.; Poloni, R.; Maximoff, S.N.; Smit, B. & Gagliardi, L., Ab Initio Carbon Capture in Open-site Metal-Organic Frameworks, *Nature Chemistry* 4, 810-816, **2012**.
  1. Martin R.L.; Willems, T.F.; **Lin, L.-C.**; Kim, J.; Swisher, J.A.; Smit, B. & Haranczyk, M., Similarity-driven Discovery of Porous Materials for Adsorption-based Separations, *ChemPhysChem* 13, 3595-3597, **2012**. \*\*\*Featured as the cover of the issue

## PRESENTATIONS

26. **Lin, L.-C.**, Computational Discovery of Nanoporous Materials for Energy-related Applications, 13<sup>th</sup> International Conference on Fundamentals of Adsorption, Cairns, Australia, **2019**. \*\*\*Invited presentation for receiving the “Triennial Award for Excellence in Publications by a Young Scientist Below 35 of the International Adsorption Society (IAS)”
25. **Lin, L.-C.**, Computational Discovery of Nanoporous Materials for Energy-related Applications, the Kang Research Group, Department of Chemical Engineering, National Taiwan University, Taiwan, **2019**.
24. **Lin, L.-C.**, Computational Discovery of Nanoporous Materials for Energy-related Applications, the Chiang Research Group, Department of Chemical Engineering, National Taiwan University of Science and Technology, Taiwan, **2019**.
23. **Lin, L.-C.**, Computational Discovery of Nanoporous Materials for Energy-related Applications, Department of Chemistry, University of South Dakota, South Dakota, USA, **2018**.
22. **Lin, L.-C.**, Computational Discovery of Nanoporous Materials for Energy-related Applications, Department of Physics, University of Maryland – Baltimore County, Maryland, USA, **2018**.

21. Zou, C. & **Lin, L.-C.\***, Computationally Investigating Zeolite Nanosheets as Pervaporation Membranes for Ethanol Extraction and the Role of Membrane Surfaces, *AIChE 2018 Annual Meeting*, Pittsburgh, USA, **2018**.
20. Yang, C.-T.; Eddin, A.C.; Poloni, R. & **Lin, L.-C.\***, Atomistic Understandings of the CO<sub>2</sub> Uptake Difference in Photo Responsive Metal-Organic Frameworks, *AIChE 2017 Annual Meeting*, Minnesota, USA, **2017**.
19. **Lin, L.-C.\***; Jamali, S.H. & Vlugt, T.J.H., Molecular Dynamics Simulations of Zeolite Nanosheets for Water Desalination, *AIChE 2017 Annual Meeting*, Minnesota, USA, **2017**.
18. **Lin, L.-C.**, Computational Discovery of Nanoporous Materials for Energy Applications, Department of Chemical and Biomedical Engineering, Cleveland State University, Ohio, USA, **2017**.
17. **Lin, L.-C.**, Computational Study of Porous Materials for Energy-Related Applications, Department of Chemical and Biomolecular Engineering, The Ohio State University, Ohio, USA, **2015**.
16. **Lin, L.-C.**, Molecular Simulations to Gas Separation Applications, Chevron Corporation, California, USA, **2014**.
15. **Lin, L.-C.**, Computational Study of Porous Materials for Gas Separations, Department of Chemical and Biomolecular Engineering, UC-Berkeley, California, USA, **2014**.
14. **Lin, L.-C.**, Computational Carbon Capture, *2014 MRS Spring Meeting*, California, USA, **2014**.
13. **Lin, L.-C.**, Molecular Simulations to Gas Separation & Storage Applications, the Grossman Research Group, MIT, Massachusetts, **2014**.
12. **Lin, L.-C. et al.**, *Ab Initio* Carbon Capture in Open-Site Metal-Organic Frameworks - Force Field Development and Its Applications, *AIChE 2013 Annual Meeting*, California, USA, **2013**.
11. **Lin, L.-C. et al.**, Computational Carbon Capture, *GRC meeting-Nanoporous Materials and its Applications*, New Hampshire, USA, **2013**.
10. **Lin, L.-C. et al.**, A New Pathway of Deriving Force Fields from Periodic Density Functional Theory Calculations, *2013 EFRC/NETL/BES/APRA-e All Hand Meeting*, California, USA, **2013**.
9. **Lin, L.-C. et al.**, Computational Carbon Capture, *EFRC PI Meeting*, Washington, D.C., USA, **2013**.
8. **Lin, L.-C. et al.**, Large-scale Computational Screening of Adsorbent Materials for Carbon Capture, *AIChE 2012 Annual Meeting*, Pittsburgh, USA, **2012**.
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