

Zhehui (Charlie) Jin

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EDUCATION AND TRAINING:

- 2003-2007 B.S.: Materials Science & Engineering, Tsinghua University, China
- 2007-2012 Ph.D.: Chemical Engineering, University of California, Riverside, U.S.A.
Supervisor: Prof. Jianzhong Wu
- 2012-2016 Researcher: Reservoir Engineering Research Institute, Palo Alto, CA, U.S.A.
Supervisor: Prof. Abbas Firoozabadi (U.S. National Academy of Engineering)

RESEARCH AND PROFESSIONAL EXPERIENCE:

- 2016-present **Tenure-Track Assistant Professor:** School of Mining and Petroleum Engineering, Department of Civil and Environmental Engineering, University of Alberta, Canada
- 2018-present **Editorial Board:** Scientific Reports
- 2012-2016 **Researcher:** Reservoir Engineering Research Institute, Palo Alto, CA, U.S.A.
- 2007-2012 **Research Assistant:** Department of Chemical and Environmental Engineering, University of California, Riverside, U.S.A.

PROFESSIONAL ACTIVITIES

Conference/Symposia Organized:

1. Session Chair, 2017 Canadian Society of Chemical Engineering Conference, Edmonton, Canada, October 2017, Co-Organizer/Co-Chair
2. “Sorptions, Phase Behavior, and Fluid Transport in Fractured Black Shales” Interpore 2018, New Orleans, U.S.A., May 2018. Co-Organizer/Co-Chair
3. Session Chair, International Conference on Properties and Phase Equilibria for Product and Process Design, Vancouver, Canada, May 2019.

Editorial Reviewer:

Served as peer reviewer for the following journals:

AICHE Journal, AIP Advances, Canadian Journal of Chemical Engineering, Carbon, Chemical Engineering Journal, Chemical Engineering Science, Computers & Mathematics with Applications, Energy and Fuels, Energy Storage Materials, Environmental Science & Technology, Fluid Phase Equilibria, Fuel, Industrial & Engineering Chemistry Research, Journal of Chemical Engineering Data, Journal of Natural Gas Science and Engineering, Journal of Petroleum Science

and Engineering, Journal of Physical Chemistry, Langmuir, Marine and Petroleum Geology, Nano Energy, Nanotechnology, SPE Journal, Transport in Porous Media, etc.

Proposal and External Reviewer:

1. Natural Sciences and Engineering Research Council of Canada (NSERC)
NSERC Discovery Grant
2. American Chemical Society Petroleum Research Fund
Doctoral New Investigator (DNI)
3. Mitacs Canada
Mitacs Accelerate Program; Mitacs Elevate Program
4. University of New South Wales
Ph.D. Thesis

Professional Affiliations:

1. American Institute of Chemical Engineers (AIChE)
2. American Chemical Society (ACS)
3. Canadian Society for Chemical Engineering (CSCHE)
4. Society of Petroleum Engineers (SPE)

INVITED PRESENTATIONS

1. *Single-Phase and Two-Phase Flows in Shale/Tight Nanoporous Media: From Molecular to Numerical Perspectives*. Key Lab of Unconventional Oil and Gas Development Workshop (Virtual), China University of Petroleum (East China), July. 2020
2. *Methane Absolute Adsorption in Shale Reservoirs: The Central Challenges Arising from Dual-Heterogeneity*. ACS Fall meeting, San Diego, USA, August. 2019
3. *Statistical Physics: A Window into Fluid Behaviors at Nanoscale*. 68th Canadian Chemical Engineering Conference, Toronto, Canada, Oct. 2018
4. *Statistical Thermodynamics: A Window into Shale Fluid Study*. China University of Petroleum, Beijing, China, June. 15. 2018
5. *Statistical Thermodynamics: A Window into Shale Fluid Study*. Tsinghua University, Beijing, China, June. 14. 2018
6. *Thermodynamic Modeling of Phase Behavior and Flow in Shale Media: A Molecular Perspective*. University of Nevada, Reno, Reno, NV, Apr. 14. 2016.
7. *Thermodynamic Modeling of Phase Behavior and Flow in Shale Media: A Molecular Perspective*. University of Tulsa, Tulsa, OK, Apr. 11. 2016.
8. *Thermodynamic Modeling of Phase Behavior and Flow in Shale Media: A Molecular Perspective*. Lawrence Livermore National Lab, Livermore, CA, Mar. 29. 2016.
9. *Thermodynamic Modeling of Phase Behavior and Flow in Shale Media: A Molecular Perspective*. University of Alberta, Edmonton, AB, Mar. 4. 2016.

HIGHLY QUALIFIED PERSONNEL (HQP) TRAINING

of Supervised PhD, MSc, Meng, Undergraduate and Visiting Students

# of Supervised PhD Students	7 (1 graduated)
# of Supervised MSc Students	2 (2 graduated)
# of Supervised Meng Students	3 (2 graduated)
# of Supervised Undergraduate Students	4 (4 graduated)
# of Supervised Visiting Students	10

HQP Oral and Poster Presentations from Dr. Jin's Group: (Underlines represent HQPs)

1. (Oral) W. Li and **Z. Jin**, *Hydrophobicity/Hydrophilicity Driven CO₂ Solubility in Kaolinite Nanopores in Relation to Carbon Sequestration*. 2020 AICHE Meeting (Virtual), Nov. 2020
2. (Oral) W. Pang and **Z. Jin**, *Analysis and Discussion of Specific Surface Area in Nanoporous Kerogen: From Molecular Simulation to Applicability of BET Theory with Different Criteria*. 2020 AICHE Meeting (Virtual), Nov. 2020
3. (Oral) W. Pang and **Z. Jin**, *Absolute Adsorption of Methane in Shale Nanoporous Media: Challenges Arising from Dual-Heterogeneity*. 2020 AICHE Meeting (Virtual), Nov. 2020
4. (Oral) Y. Nan and **Z. Jin**, *Roles of Alcohol as A Cosurfactant at Brine-Oil Interface under A Typical Reservoir Condition*. 2020 AICHE Meeting (Virtual), Nov. 2020
5. (Oral) W. Li and **Z. Jin**, *Effects of Salinity and N-, S-, and O-Bearing Polar Components on Light Oil-Brine Interfacial Properties from Molecular Perspectives*. 2020 AICHE Meeting (Virtual), Nov. 2020
6. (Oral) Y. Nan and **Z. Jin**, *Slip Length of Methane Flow under Shale Reservoir Conditions: Effect of Pore Size and Pressure*. 2020 AICHE Meeting (Virtual), Nov. 2020
7. (Oral) W. Li and **Z. Jin**, *CO₂ Solubility in Water Confined by Kerogen Nanopore in Relation to CO₂ Sequestration in Depleted Shale Reservoirs: A Molecular Dynamics Simulation Study*. 2020 AICHE Meeting (Virtual), Nov. 2020
8. (Oral) M. Zhang and **Z. Jin**, *Molecular Dynamics Study on the Intercalation Behaviors of Polyethylene Glycols into Montmorillonite Interlayer*. 2020 AICHE Meeting (Virtual), Nov. 2020
9. (Oral) M. Zhang and **Z. Jin**, *The Structural Properties of Micropollutants in Activated Carbons in Relation to Greywater Treatment: A Molecular Dynamics Study*. 2020 AICHE Meeting (Virtual), Nov. 2020
10. (Oral) M. Zhang and **Z. Jin**, *Molecular Insights into Adsorption Behavior of Naphthenic Acids in Carbonaceous Materials*. 2020 AICHE Meeting (Virtual), Nov. 2020
11. (Oral) W. Pang and **Z. Jin**, *Methane Absolute Adsorption in Kerogen Nanoporous Media With Realistic Continuous Pore Size Distributions*. Interpore Meeting (Virtual), Sep. 2020
12. (Oral) M. Zhang and **Z. Jin**, *The Structural Properties of Micropollutants in Activated Carbons in Relation to Greywater Treatment: A Molecular Dynamics Study*. 2020 AICHE Meeting (Virtual), Nov. 2020
13. (Oral) W. Zhang, Q. Feng and **Z. Jin**, *CO₂-Regulated Octane Flow in Calcite Nanopores from Molecular Perspectives*. Interpore Meeting (Virtual), Sep. 2020

14. (Oral) W. Li and **Z. Jin**, *Effects of Salinity and N-, S-, and O-Bearing Polar Components on Light Oil-Brine Interfacial Properties from Molecular Perspectives*. Interpore Meeting (Virtual), Sep. 2020
15. (Oral) W. Li and **Z. Jin**, *Hydrophobicity/Hydrophilicity Driven CO₂ Solubility in Kaolinite Nanopores in Relation to Carbon Sequestration*. Interpore Meeting (Virtual), Sep. 2020
16. (Oral) S. Zhan, Y. Su, **Z. Jin**, W. Wang, and L. Li, *Oil-Water Two-Phase Flow Behavior in Shale Inorganic Nanopores: From Molecule Level to Theoretical Mathematical Model*. SPE/AAPG/SEG Unconventional Resources Technology Conference (Virtual), July. 2020
17. (Poster) Y. Wang, W. Pang and **Z. Jin**, *Stability Limit of Fluids under Weakly-Adsorbing Confinement: An Engineering Density Functional Theory Study*. International Conference on Properties and Phase Equilibria for Product and Process Design, Vancouver, Canada, May. 2019
18. (Poster) W. Li and **Z. Jin**, *Effect of Multi-valent Ions and Their Concentrations on the Interfacial Tensions between Natural Gas and Brine from Molecular Dynamics Simulations*. International Conference on Properties and Phase Equilibria for Product and Process Design, Vancouver, Canada, May. 2019
19. (Oral) W. Pang and **Z. Jin**, *Revisiting Methane Absolute Adsorption in Organic Nanopores from Molecular Simulation and Ono-Kondo Lattice Model*. 68th Canadian Chemical Engineering Conference, Toronto, Canada, Oct. 2018
20. (Poster) W. Pang and **Z. Jin**, *Ono-Kondo Lattice Model for Propane Multilayer Adsorption in Organic Nanopores in Relation to Shale Gas*. 68th Canadian Chemical Engineering Conference, Toronto, Canada, Oct. 2018
21. (Poster) Y. Zhao, Y. Wang and **Z. Jin**, *Breaking the Myth about Bubble Point Pressure of Nano-Confined Hydrocarbon Mixtures in Relation to Shale/Tight Oil Recovery: From Statistical Thermodynamics*. 68th Canadian Chemical Engineering Conference, Toronto, Canada, Oct. 2018
22. (Oral) Y. Wang and **Z. Jin**, *Effect of Pore Size Distributions on The Phase Behavior of Nano-Confined Hydrocarbons in Relation to Shale Gas Recovery from Density Functional Theory*. 68th Canadian Chemical Engineering Conference, Toronto, Canada, Oct. 2018
23. (Oral) W. Li and **Z. Jin**, *Molecular Dynamics Simulations of Natural Gas-Water Interfacial Tensions over Wide Range of Pressures*. 68th Canadian Chemical Engineering Conference, Toronto, Canada, Oct. 2018
24. (Oral) W. Pang and **Z. Jin**, *Accurate Characterization of Methane and Propane Absolute Adsorption from Ono-Kondo Lattice Model in Relation to Shale Gas*. International Workshop on Molecular Simulation, Shanghai, China, August. 2018
25. (Oral) W. Pang, **Z. Jin**, Y. He, and C. Yan, *Tackling Challenges in Estimation of Methane Absolute Adsorption in Kerogen Nanoporous Media from Molecular and Analytical Perspectives*. International Workshop on Molecular Simulation, Shanghai, China, August. 2018

26. (Oral) X. Hu, Y. Tian, H. Deng, and **Z. Jin**, *Molecular Simulation of Competitive Adsorption Behaviors of CO₂/CH₄ Mixtures on Shale Clay Minerals*. Interpore 2018, New Orleans, United States, May. 2018
27. (Oral) Y. Tian and **Z. Jin**, *Accurate Characterization of Absolute Adsorption in Clay Minerals in Relation to Shale Gas from Molecular Perspective*. 67th Canadian Chemical Engineering Conference, Edmonton, AB, Canada, Oct. 22-25, 2017
28. (Oral) Y. Liu, **Z. Jin** and H. Li, *Comparison of PR-EOS with Capillary Pressure Model with Engineering Density Functional Theory on Describing the Phase Behavior of Confined Hydrocarbons*. 2017 SPE Annual Technical Conference and Exhibition, San Antonio, TX, Oct. 9-11, 2017

Students' Awards (Scholarships, fellowships, and travel awards)

Shiyuan Zhan	Outstanding Graduate Student Research Award, China University of Petroleum East China, 2020 (Note: only 10 awardees throughout the university per year)
Shiyuan Zhan	National Outstanding Graduate Student Fellowship (China), 2020
Yingnan Wang	Doctoral Recruitment Scholarship, University of Alberta, 2019
Wenhui Li	Future Energy Systems Opportunity Fund, 2019
Wanying Pang	Future Energy Systems Opportunity Fund, 2019
Yinuo Zhao	FGSR Graduate Travel Award, University of Alberta, 2018
Yingnan Wang	FGSR Graduate Travel Award, University of Alberta, 2018
Wanying Pang	GSA Academic Travel Award, University of Alberta, 2018
Wenhui Li	GSA Academic Travel Award, University of Alberta, 2018
Yiling Nan	Doctoral Recruitment Scholarship, University of Alberta, 2018
Mingshan Zhang	China Scholarship Council Study Abroad Scholarship, 2018
Wenhui Li	Doctoral Recruitment Scholarship, University of Alberta, 2017
Wenhui Li	China Scholarship Council Study Abroad Scholarship, 2017

PEER-REVIEWED JOURNAL PUBLICATIONS

“*” *corresponding author*, “†” *co-first author*, Underlines: HQPs

➤ *Google Scholar Citation: > 2100*

Year 2021

1. Deng, Z., W. Pang, **Z. Jin**, and X. Wang*, *Pt-Oxygen Interaction Evolution of Pt₃Co Nanowires by Mo Doping Enabling Enhanced Oxygen Reduction Reaction Performance*. **Submitted**.
2. Zhang, X.[†], Q. Jin[†], Y. Nan[†], L. Hou, B. Li, X. Chen, **Z. Jin**, X. Zhang, J. Huang, and Q. Zhang*, *Electrolyte Structure Regulation for Stabilizing Polysulfide Intermediates in Practical Lithium-Sulfur Batteries*. **Submitted**.
3. Zhang, M., W. Li, and **Z. Jin***, *Structural Properties of Deprotonated Naphthenic Acids Immersed in Water in Pristine and Hydroxylated Carbon Nanopores from Molecular Perspectives*. **Under Revision**.

4. Zhao, Y., C. Lu, and **Z. Jin***, *Revisiting the Comparison between Density Functional Theory and Equation-of-State Based Models on Phase Behavior of Hydrocarbon Mixtures Under Nanoconfinement: Canonical Ensemble*. **Under Revision**.
5. Wang, Y. and **Z. Jin***, *Hydrocarbon Mixture and CO₂ Adsorption in A Nanopore-Bulk Multiscale System in Relation to CO₂ Enhanced Shale Gas Recovery*. **Accepted**.
6. Zhao, Y. and **Z. Jin***, *Hydrocarbon Mixture Phase Behavior in Multi-Scale Systems in Relation to Shale Oil Recovery: The Effect of Heterogeneous Pore Size Distributions*. **Under Revision**.
7. Li, W., Y. Nan, Q. You* and **Z. Jin***, *CO₂ Solubility in Brine in Silica Nanopores in Relation to Geological CO₂ Sequestration in Tight Formations: Effect of Salinity and pH*. *Chemical Engineering Journal*, 2021. **Accepted**.
8. Zhang, W., Q. Feng*, S. Wang, X. Xing, and **Z. Jin***, *CO₂-Regulated Octane Flow in Calcite Nanopores from Molecular Perspectives*. *Fuel*, 2021. **286**: 119299.
9. Shardt, N., Y. Wang, **Z. Jin**, and J. A. W. Elliot*, *Surface Tension as A Function of Temperature and Composition for A Broad Range of Mixtures*. *Chemical Engineering Science*, 2021. **230**: 116095.
10. Zhang, M., H. Mao, and **Z. Jin***, *Molecular Dynamic Study on Structural and Dynamic Properties of Water, Counter-ions and Polyethylene Glycols in Na-Montmorillonite Interlayer*. *Applied Surface Science*, 2021. **536**: 147700.

Year 2020

11. Zhan, Y., P. Shi, X. Zhang, F. Ding, J. Huang*, **Z. Jin**, R. Xiang, X. Liu, and Q. Zhang*, *The Insights of Lithium Metal Plating/Stripping in Porous Hosts: Progress and Perspectives*. *Energy Technology*, 2020. **Accepted**.
12. Li, W., M. Zhang, Y. Nan, W. Pang, and **Z. Jin***, *Molecular Dynamics Study on CO₂ Storage in Water-Filled Kerogen Nanopores in Shale Reservoirs: Effects of Kerogen Maturity and Pore Size*. *Langmuir*, 2020. **Accepted**.
13. Pang, W. and **Z. Jin***, *Methane Absolute Adsorption in Kerogen Nanoporous Media With Realistic Continuous Pore Size Distributions*. *Energy & Fuels*, 2020. **34 (10)**: p. 12158-12172.
14. Wang, H., J. M. Shaw*, and **Z. Jin***, *Discontinuous Displacement at Solvent-Immobile Hydrocarbon Interfaces*. *Energy & Fuels*, 2020. **34 (8)**: p. 9392-9400.
15. Lu, C., **Z. Jin**, and H. Li*, *Determination of Hildebrand Solubility Parameter for Pure Hydrocarbons by Incorporating Temperature-Dependent Volume Translation into Peng-Robinson Equation of State*. *Journal of Supercritical Fluids*, 2020. **164**: 104945.
16. Zhou, J., **Z. Jin***, and K. Luo*, *The Role of Brine in Gas Adsorption and Dissolution in Kerogen Nanopores for Enhanced Gas Recovery and CO₂ Sequestration*. *Chemical Engineering Journal*, 2020. **399**: 125704.
17. Wang, Y., N. Shardt, C. Lu, H. Li, J. Elliot and **Z. Jin***, *Validity of the Kelvin Equation and the Equation-of-State-with-Capillary-Pressure Model for the Phase Behavior of a Pure Component under Nanoconfinement*. *Chemical Engineering Science*, 2020. **226**: 115839.

18. Li, W., Y. Nan, Z. Zhang, Q. You*, and **Z. Jin***, *Hydrophilicity/Hydrophobicity Driven CO₂ Solubility in Kaolinite Nanopores in Relation to Carbon Sequestration*. Chemical Engineering Journal, 2020. **398**: 125449.
19. Zhan, S., Y. Su*, **Z. Jin***, W. Wang, M. Cai, L. Li, and Y. Hao, *Molecular Insight into the Boundary Conditions of Water Flow in Clay Nanopores*. Journal of Molecular Liquids, 2020. **311**: 113292.
20. Nan, Y., W. Li, and **Z. Jin***, *Roles of Alcohol as a Cosurfactant at Brine-Oil Interface under a Typical Reservoir Condition*. Langmuir, 2020. **36 (19)**: p. 5198-5207.
21. Zhan, S., Y. Su*, **Z. Jin***, M. Zhang, W. Wang, Y. Hao, and L. Li, *Study of Liquid-Liquid Two-Phase Flow in Hydrophilic Nanochannels by Molecular Simulations and Theoretical Modeling*. Chemical Engineering Journal, 2020. **395**: 125053.
22. Jiang, P., H. Wu, L. Qing, X. Xu, **Z. Jin**, L. Yang, and S. Zhao*, *A Wetting Transition of Ionic Substrate by Modulating Surface Charge Distribution*. Langmuir, 2020. **36 (13)**: p. 3667-3675.
23. Chen, W., C. Zhao, B. Li, Q. Jin, X. Zhang, T. Yuan, X. Zhang, **Z. Jin**, S. Kaskel, and Q. Zhang*, *A Mixed Ether Electrolyte for Lithium Metal Anode Protection in Working Lithium-Sulfur Batteries*. Energy & Environmental Materials, 2020. **3**: 160-165.
24. Li, W., Y. Nan, Q. You*, Q. Xie, and **Z. Jin***, *Effects of Salts and Silica Nanoparticles on Oil-Brine Interfacial Properties under Hydrocarbon Reservoir Conditions: A Molecular Dynamics Simulation Study*. Journal of Molecular Liquids, 2020. **305**: 112860.
25. Zhou, J., **Z. Jin***, and K. Luo*, *Insights Into Recovery of Multi-Component Shale Gas by CO₂ Injection: A Molecular Perspective*. Fuel, 2020. **267**: 117247.
26. Ding, S., M. Li, W. Pang, B. Hua, N. Duan, Y. Zhang, S. Zhang, **Z. Jin***, and J. Luo*, *A-site Deficient Perovskite with Nano-Socketed Ni-Fe Alloy Particles as Highly Active and Durable Catalyst for High-Temperature CO₂ Electrolysis*. Electrochimica Acta, 2020. **335**: 135683.
27. Chen, J., X. Zhang, B. Li, X. Wang, P. Shi, W. Zhu, A. Chen, **Z. Jin**, R. Xiang, J. Huang*, and Q. Zhang*, *The Origin of Sulfuryl-Containing Components in SEI from Sulfate Additive for Stable Cycling of Ultrathin Lithium Metal Anodes*. Journal of Energy Chemistry, 2020. **47**: p. 128-131
28. Chen, L., Z. Huang, W. Pang, **Z. Jin**, Y. Li*, and C. Wang*, *Dual Interface Layers for Solid-State Li Metal Battery with Low Interfacial Resistance and Small Polarization Based on Garnet Electrolyte*. Electrochimica Acta, 2020. **330**: 135352.
29. Zhan, S., Y. Su*, **Z. Jin***, W. Wang, and L. Li, *Effect of Water Film on Oil flow in Quartz Nanopores from Molecular Perspectives*. Fuel, 2020. **262**: 116560.
30. Nan, Y., W. Li, and **Z. Jin***, *Slip Length of Methane Flow under Shale Reservoir Conditions: Effect of Pore Size and Pressure*. Fuel, 2020. **259**: 116237.
31. Zhang, M., S. Zhan, and **Z. Jin***, *Recovery Mechanisms of Hydrocarbon Mixtures in Organic and Inorganic Nanopores During Pressure Drawdown and CO₂ Injection from Molecular Perspectives*. Chemical Engineering Journal, 2020. **382**: 122808.

Year 2019

32. Zhao, Y. and **Z. Jin***, *Hydrocarbon Phase Behaviors in Shale Nanopore-Fracture Model: Multi-scale, Multi-component and Multi-Phase*. SPE Journal, 2019. **24 (6)**: p. 2526-2540.
33. Li, W., Y. Nan, X. Wen, W. Wang*, and **Z. Jin***, *Effects of Salinity and N-, S-, and O-Bearing Polar Components on Light Oil-Brine Interfacial Properties from Molecular Perspectives*. Journal of Physical Chemistry C, 2019. **123 (38)**: p. 23520-23528.
34. Hu, X., H. Deng*, C. Lu, Y. Tian, and **Z. Jin***, *Characterization of CO₂/CH₄ Competitive Adsorption in Various Clay Minerals in Relation to Shale Gas Recovery from Molecular Simulation*. Energy and Fuels, 2019. **33 (9)**: p. 8202-8214.
35. Liu, H., X. Cheng, **Z. Jin**, R. Zhang, G. Wang, L. Chen, Q. Liu, J. Huang*, and Q. Zhang* *Recent Advances in Understanding Dendrite Growth on Alkali Metal Anodes*. Energychem, 2019. **1 (1)**: 100003.
36. Pang, W., Y. Ye, and **Z. Jin***, *Assessment of Various Approaches in the Prediction of Methane Absolute Adsorption in Kerogen Nanoporous Media*. Energy and Fuels, 2019. **33 (7)**: p. 6258-6263.
37. Huang, Z., W. Pang, L. Peng, **Z. Jin**, N. S. Grundish, Y. Li*, and C. Wang*, *Dopamine Modified Li_{6.4}La₃Zr_{1.4}Ta_{0.6}O₁₂/PEO Solid-State Electrolyte: Enhanced Thermal and Electrochemical Properties*. Journal of Materials Chemistry A, 2019. **7**: p. 16425-16436.
38. Zhou, J., Z. Jin*, and KH. Luo*, *Effects of Moisture Contents on Shale Gas Recovery and CO₂ Sequestration*. Langmuir, 2019. **35 (26)**: p. 8716-8725.
39. Wang, Y. and **Z. Jin***, *Effect of pore size distribution on hydrocarbon mixtures adsorption in shale nanoporous media from engineering density functional theory*. Fuel, 2019. **254**: 115650.
40. Li, W. and **Z. Jin***, *Effect of Ion Concentration and Multivalence on Methane-Brine Interfacial Tension and Phenomena from Molecular Perspectives*. Fuel, 2019. **254**: 115657.
41. Pang, W., Y. He, C. Yan, and **Z. Jin***, *Takling the challenges in the estimation of methane absolute adsorption in kerogen nanoporous media from molecular and analytical approaches*. Fuel, 2019. **242**: p. 687-698.
42. Lu, C., Z. Jin, and HA. Li*, *A two-phase flash algorithm with the consideration of capillary pressure at specified mole numbers, volume and temperature*. Fluid Phase Equilibria, 2019. **485**: p. 67-82.
43. Zhang, Y., M. Gao, Q. You*, H. Fan, W. Li, Y. Liu, J. Fang, G. Zhao, **Z. Jin**, and C. Dai*, *Smart mobility control agent for enhanced oil recovery during CO₂ flooding in ultra-low permeability reservoirs*. Fuel, 2019. **241**: p. 442-450.
44. Li, W. and **Z. Jin***, *Molecular dynamics simulations of natural gas-water interfacial tensions over wide range of pressures*. Fuel, 2019. **236**: p. 480-492.
45. Jatukaran, A., J. Zhong, A. Abedidi, A. Sherbatian, Y. Zhao, **Z. Jin**, F. Mostowfi, and D. Sinton*, *Natural gas vaporization in a nanoscale throat connected model of shale: Multi-scale, Multi-component and Multi-phase*. Lab on a Chip, 2019. **19**: p. 272-280
46. Pang, W. and **Z. Jin***, *Revisiting Methane Absolute Adsorption in Organic Nanopores from Molecular Simulation and Ono-Kondo Lattice Model*. Fuel, 2019. **235**: p. 339-349

47. Pang, W. and **Z. Jin***, *Ono-Kondo Lattice Model for Propane Multilayer Adsorption in Organic Nanopores in Relation to Shale Gas*. Fuel, 2019. **235**: p. 158-166

Year 2018

48. Hua, B., M. Li, W. Pang, W. Tang, S. Zhao, **Z. Jin**, Y. Zeng, B.S. Amirkhiz, and J. Luo*, *Activating p-Blocking Centers in Perovskite for Efficient Water Splitting*. Chem, 2018. **4 (12)**: p. 2902-2916.
49. Yu, X., W. Tang, T. Zhao, **Z. Jin**, S. Zhao*, and H. Liu*, *Confinement Effect on Molecular Conformation of Alkanes in Water-filled Cavities: A Combined Quantum/Classical DFT Study*. Langmuir, 2018. **34 (45)**: p. 13491-13496.
50. Zhao, Y., Y. Wang, J. Zhong, Y. Xu, D. Sinton, and **Z. Jin***, *Bubble Point Pressures of Hydrocarbon Mixtures in Multiscale Volumes from Density Functional Theory*. Langmuir, 2018. **34 (46)**: p. 14058-14068.
51. Zhong, J., Y. Zhao, C. Lu, Y. Xu, **Z. Jin**, F. Mostowfi, and D. Sinton*, *Nanoscale Phase Measurement for the Shale Challenge: Multi-component Fluids in Multi-scale Volumes*. Langmuir, 2018. **34 (34)**: p. 9927-9935.
52. Liu, Y., HA. Li*, Y. Tian, **Z. Jin**, and H. Deng*, *Determination of the absolute adsorption/desorption isotherms of CH₄ and n-C₄H₁₀ on shale from a nano-scale perspective*. Fuel, 2018. **218**: p. 67-77.
53. **Jin, Z.***, *Bubble/dew point and hysteresis of hydrocarbons in nanopores from molecular perspective*. Fluid Phase Equilibria, 2018. **458**: p. 177-185.
54. Liu, Y., **Z. Jin***, and HA. Li, *Comparison of PR-EOS with capillary pressure model with engineering density functional theory on describing the phase behavior of confined hydrocarbons*. SPE Journal, 2018. **23 (5)**: p. 1784-1797.

Year 2017

55. Tian, Y., C. Yan, and **Z. Jin***, *Characterization of methane excess and absolute adsorption in various clay nanopores from molecular simulation*. Scientific Reports, 2017. **7 (1)**: 12040.
56. **Jin, Z.***, *Effect of Nano-Confinement on High Pressure Methane Flow Characteristics*. Journal of Natural Gas Science and Engineering, 2017. **45**: p. 575-583.

Prior to the University of Alberta

57. **Jin, Z.** and A. Firoozabadi*, *Phase Behavior and Flow in Shale Nanopores from Molecular Simulations*. Fluid Phase Equilibria, 2016. **430**: p. 156-168.
58. **Jin, Z.** and A. Firoozabadi*, *Thermodynamic Modeling of Phase Behavior in Shale Media*. SPE Journal, 2016. **21(01)**: p. 190-207.
59. **Jin, Z.** and A. Firoozabadi*, *Flow of Methane in Shale Nanopores at Low and High Pressure by Molecular Dynamics Simulations*. Journal of Chemical Physics, 2015. **143(10)**: p. 104315.
60. Li, Z., **Z. Jin**, and A. Firoozabadi*, *Phase behavior and adsorption of pure substances and mixtures and characterization in nanopore structures by density functional theory*. SPE Journal, 2014. **19(6)**: p. 1096-1109.

61. **Jin, Z.** and A. Firoozabadi*, *Effect of Water on Methane and Carbon Dioxide Sorption in Clay Minerals by Monte Carlo Simulations*. *Fluid Phase Equilibria*, 2014. **382**: p. 10-20.
62. **Jin, Z.** and A. Firoozabadi*, *Methane and carbon dioxide adsorption in clay-like slit pores by Monte Carlo simulations*. *Fluid Phase Equilibria*, 2013. **360**: p. 456-465.
63. Jiang, D.-e.*, **Z. Jin**, D. Henderson, and J. Wu*, *Solvent Effect on the Pore-Size Dependence of an Organic Electrolyte Supercapacitor*. *The Journal of Physical Chemistry Letters*, 2012. **3**(13): p. 1727-1731.
64. Henderson, D.*, D.-e. Jiang, **Z. Jin**, and J. Wu*, *Application of Density Functional Theory To Study the Double Layer of an Electrolyte with an Explicit Dimer Model for the Solvent*. *The Journal of Physical Chemistry B*, 2012. **116**(36): p. 11356-11361.
65. **Jin, Z.**, J. Kim, and J. Wu*, *Shape Effect on Nanoparticle Solvation: A Comparison of Morphometric Thermodynamics and Microscopic Theories*. *Langmuir*, 2012. **28**(17): p. 6997-7006.
66. **Jin, Z.** and J. Wu*, *Density functional theory for encapsidated polyelectrolytes: A comparison with Monte Carlo simulation*. *The Journal of Chemical Physics*, 2012. **137**(4): p. 044905.
67. Wu, J.*, T. Jiang, D.-e. Jiang*, **Z. Jin**, and D. Henderson*, *A classical density functional theory for interfacial layering of ionic liquids*. *Soft Matter*, 2011. **7**(23): p. 11222-11231.
68. Jiang, D.-e.*, **Z. Jin**, and J. Wu*, *Oscillation of Capacitance inside Nanopores*. *Nano Letters*, 2011. **11**(12): p. 5373-5377.
69. Henderson, D.*, S. Lamperski, **Z. Jin**, and J. Wu, *Density Functional Study of the Electric Double Layer Formed by a High Density Electrolyte*. *The Journal of Physical Chemistry B*, 2011. **115**(44): p. 12911-12914.
70. Zhao, S., **Z. Jin**, and J. Wu*, *New Theoretical Method for Rapid Prediction of Solvation Free Energy in Water*. *The Journal of Physical Chemistry B*, 2011. **115**(21): p. 6971-6975.
71. **Jin, Z.** and J. Wu*, *Hybrid MC–DFT Method for Studying Multidimensional Entropic Forces*. *The Journal of Physical Chemistry B*, 2011. **115**(6): p. 1450-1460.
72. **Jin, Z.**, Y. Tang, and J. Wu*, *A perturbative density functional theory for square-well fluids*. *The Journal of Chemical Physics*, 2011. **134**(17): p. 174702.
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