

Department: School of Chemical Engineering

Professional field: Chemical Engineering and Technology

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Profile

Education

2007: PhD, Physical Chemistry, Ecole Normale Supérieure de Lyon, France.

2004: MS, Theoretical Physics, Hunan University, China.

2002: BS (with honor), Applied Physics, Hunan University, China.

2002: Diploma in Computer Science, Hunan University, China.

Academic Experience

2017-present: Professor, School of Chemical Engineering, ECUST, China.

2012-2017: Associate professor, School of Chemical Engineering, ECUST, China.

2009-2012: Postdoctoral Research, Chemical Engineering Department, University of California at Riverside, USA.

2007-2009: Postdoctoral Research, Chemistry Department, Ecole Normale Supérieure, Paris, France.

Research Field

Interface Statistical thermodynamics: Development of statistical Density functional theory and computer modelling methods, Dedicated to the thermodynamics of micro-nano interface systems, Study on kinetics and interfacial reaction

Research results and selected published papers

- 1.X.Y. Song, H. Guo, J.B. Tao, S.L. Zhao*, X. Han and H.L. Liu. Encapsulation of single-walled carbon nanotubes with asymmetric pyrenyl-gemini surfactants. *Chemical Engineering Science*, 187, 406-414 (2018)
- 2.X.Y. Song, H. Guo, J.B. Tao, S.L. Zhao*, X. Han and H.L. Liu*. Design of tunable-size 2D nanopore membranes from self-assembled amphiphilic nanosheets using dissipative particle dynamics simulations. *Chemical Engineering Science*, 189, 75–83 (2018)
- 3.J.B. Tao, X.Y. Song, W. Chen, S.L. Zhao* and H.L. Liu*. Thermostat effect on water transport dynamics across CNT membranes. *Molecular Simulation*, DOI: 10.1080/08927022.2018.1475740 (2018)
- 4.J.B. Tao, X.Y. Song, T. Zhao, S.L. Zhao* and H.L. Liu*. Confinement effect on water transport in CNT membranes. *Chemical Engineering Science*, DOI: 10.1016/j.ces.2018.05.018 (2018)
- 5.X.C. Yu, J. Zhang, S.L. Zhao*, X.H. Yu*, and H.L. Liu. An investigation into the effect of gas adsorption on safety valve set pressure variations. *Chemical Engineering Science*, 188, 170-178 (2018)
- 6.W.Q. Tang, J. Xuan, H.Z. Wang*, S.L. Zhao* and H.L. Liu. First-principles investigation of aluminum intercalation and diffusion in TiO₂ materials: Anatase versus rutile. *Journal of Power Sources*, 384, 249-255 (2018)
- 7.M. Liu, W.Q. Tang, Y.S. Xu, H.B. Yu, H.F. Yin*, S.L. Zhao*, S.H. Zhou*. Pd-SnO₂/Al₂O₃ heteroaggregate nanocatalysts for selective hydrogenations of p-nitroacetophenone and p-nitrobenzaldehyde. *Applied Catalysis A: General*, 549: 273-279 (2018)
- 8.Y.H. Dong, R. An, S.L. Zhao, W. Cao, L.L. Huang, W. Zhuang, L.H. Lu, and X.H. Lu*. Molecular interactions of protein with TiO₂ by AFM measured adhesion force. *Langmuir*, 33(42):11626 (2017)
- 9.H.G. Wu, Y. Li, D. Kadirov, S.L. Zhao*, X.H. Lu, and H.L. Liu. Efficient Molecular Approach to Quantifying Solvent-Mediated Interactions. *Langmuir*, 33, 11817-11824 (2017)
- 10.Z.Q. Fang, X.C. Yu, W.Q. Tang, X.H. Yu*, S.L. Zhao* and S.T. Tu. “Denitration by oxidation-absorption with polypropylene hollow fiber membrane contactor”. *Applied Energy*, 206, 858-868 (2017)
- 11.M.M. Ma, S.L. Zhao*, Z.L. Xu* and H.L. Liu. “Microscopic Insights into the Efficiency of Capacitive Mixing Process”. *AIChE Journal* 63(6) 1785-1791 (2017)
- 12.M.M. Liu, W.Q. Tang, Z.H. Xie, H.B. Yu, H.F. Yin, Y.S. Xu*, S.L. Zhao* and S.H. Zhou*. “Design of Highly Efficient Pt-SnO₂ Hydrogenation Nanocatalysts Using Pt@Sn Core-shell Nanoparticles”, *ACS Catalysis*, 7:1583-1591 (2017)
- 13.Y.F. Hu, X.C. Yu, J.B. Tao, Y. Liu, S.L. Zhao* and H.L. Liu, “Blocking effect of benzene-like fluid transport in nanoscale block-pores”, *Molecular Simulation*, 43(7): 526-533 (2017)
- 14.W. Yu, J.B. Tao, X.H. Yu*, S.L. Zhao*, S.T. Tu and H.L. Liu, “A Microreactor with Superhydrophobic Pt-Al₂O₃ Catalyst Coating concerning Oxidation of Hydrogen Off-gas from Fuel Cell”. *Applied Energy*. 185,1233-1244 (2017)
- 15.S.L. Zhao, Y.F. Hu, X.C. Yu, Y. Liu Z.S. Bai and H.L. Liu, “Surface Wettability Effect on Fluid Transport in Nanoscale Slit Pores”, *AIChE Journal*, 63(5): 1704-1714 (2016)
- 16.S.L. Zhao, B.C. Zhan, Y.F. Hu, Z.Y. Fan, M. Pera-Titus*, and H.L. Liu*. “Dynamics of Pickering emulsions in the presence of an interfacial reaction: a simulation study”. *Langmuir*, 32, 12975-12985 (2016)
- 17.Y.F. Hu, L.L. Huang, S.L. Zhao, H.L. Liu and K.E. Gubbins*. Effect of Confinement in Nano-Porous Materials on the Solubility of a Supercritical Gas, *Molecular Physics*. 114(22), 3294-3306 (2016)
- 18.W. Chen, S.L. Zhao, M. Holovko, X.S. Chen, and W. Dong*. “Scaled Particle Theory for Multicomponent Hard Sphere Fluids Confined in Random Porous Media”. *J. Phys. Chem. B*, 120, 5491–5504 (2016)
- 19.J.L. Tang, C. Cai, X.X. Ming, X.H. Yu*, S.L. Zhao*, S.T. Tu and H.L. Liu, Morphology and stress at silicon-glass interface in anodic bonding. *Applied Surface Science*, 387, 139-148 (2016)
- 20.M.M. Ma, S.L. Zhao* and Z.L. Xu*, “Investigation of dielectric decrement and correlation effects on electric double-layer capacitance by self-consistent field model”, *Communications in Computational Physics*. 20(2), 441-458 (2016)
- 21.S.L. Zhao, Y. Liu, X.Q. Chen, Y.X. Lu, H.L. Liu* and Y. Hu, “Unified Framework of Multi-scale Density Functional Theories and Its Recent Applications”. *ACHEM: Mesoscale Modeling in Chemical Engineering II*. Chapter 1 Volume 47, 2015, Pages 1–83, Elsevier Publisher
- 22.Y.S. Xu, K.H. Shi, S.L. Zhao* X.H. Guo and J. Zhang*, “Block Length Determines the Adsorption Dynamics Mode of Triblock Copolymers to a Hydrophobic Surface”. *Chemical Engineering Science*. 142:180-189 (2016)
- 23.Y. Liu, F.Y. Guo, J. Hu, S.L. Zhao, H.L. Liu* and Y. Hu, “Screening of Desulfurization Adsorbent in Metal-organic Frameworks: A Classical Density Functional Approach”. *Chemical Engineering Science*, 137, 170-177 (2015)
- 24.Y. Liu, S.L. Zhao, H.L. Liu* and Ying Hu, “High-throughput and Comprehensive Prediction of H₂ Adsorption in Metal-Organic Frameworks under Various Conditions”. *AIChE Journal*, 61(9), 2951-2957 (2015)
- 25.L.W. Fu, X.W. Shi, H.L. Zhao, S.L. Zhao*, Z.S. Bai and H.L. Liu, “Two Chelating Polymeric Beads and Their Adsorption Properties Toward Trace Co (II) from Wastewater”. *Journal of Multidisciplinary Engineering Science and Technology*, 2(8), 2522 (2015)
- 26.B.C. Zhan, K. H. Shi, Z.X. Dong, W.J. Lv, S.L. Zhao*, X. Han* and H.L. Liu, “Coarse-Grained Simulation of Polycation/DNA-like Complexes: Role of Neutral Block”. *Molecular Pharmaceutics*. 12(8), 2834 (2015)
- 27.Y.F. Hu, W.J. Lv, S.L. Zhao*, Y.Z. Shang, H.L. Liu* and H.L. Wang, “Effect of Surfactant SDS on DMSO Transport across Water/Hexane Interface by Molecular Dynamics Simulation”, *Chemical Engineering Science*, 134, 813-822 (2015)
- 28.Z.H. Liu, W.J. Lv, S.L. Zhao*, Y.Z. Shang, C.J. Peng, H.L. Wang, and H.L. Liu. “Effects of Hydrophilicity or Hydrophobicity of Neutral Block on Structure Formation of Block Polyelectrolyte/Surfactants Complex: A Molecular Dynamics Simulation Study”, *Computational Condensed Matter*. 2, 16-24 (2015)
- 29.K.H. Shi, C. Lian, Z.S. Bai, S.L. Zhao*, H.L. Liu, “Dissipative particle dynamics study of the water/benzene/caprolactam system in the absence or presence of non-ionic surfactants”. *Chemical Engineering Science*, 122 185–196 (2015)
- 30.C.Z. Qiao, W.J. Liu, L.W. Fu, Z. Bai, S.L. Zhao*, HL Liu. Theoretical study on adsorption of nanoparticles in dilute concentration under shear flow. *CIESC Journal (化工学报)*, 66(1): 132-141 (2015)