

## 乔智威个人简介

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### 基本情况:

乔智威，男，1986年生，工学博士，教授，硕士生导师，广东省青年拔尖人才，广州市高层次人才。

### 联系方式:

E-mail: qzw3140cn@126.com;

### 教育经历:

2008/9-2013/9 华南理工大学，化学与化工学院，化学工程专业，获工学博士学位

2011/9-2012/9 美国西北大学，化工系，化学工程专业，联合培养博士生

2004/9-2008/6 华南理工大学，化学与化工学院，化学工程与工艺专业，获工学学士学位

**工作经历:**

2018/2-至今 任广州大学化学化工学院化工系专任教师, 硕士生导师, 从事教学和科学研究

2013/9-2018/2 分别在华南理工大学制浆造纸工程国家重点实验室、化学与化工学院和新加坡国立大学工程学院化工系从事博士后研究

**科研方向:**

目前主要从事化工材料高通量计算与智能设计。通过计算机分子模拟手段高通量筛选和人工智能技术自动设计新型多孔材料, 如金属-有机框架材料(MOFs)、分子筛、聚合物材料等; 使用大数据分析建立材料的成分-结构-性能三维关系, 并择优进行实验合成。

**科研项目:****主持科研项目11项:**

[11] 广东省人才计划——青年拔尖人才, 人工智能自动批量设计环保新材料, 2020.01-2024.12, 250万元;

[10] 国家自然科学基金项目, 面上项目, 基于高通量计算和人工智能的MOF吸附剂自动设计方法的研究, 2020.01-2023.12, 65万元;

[9] 国家自然科学基金项目, 面上项目, 高效手性分离性能的单一手性金属-有机骨架材料的分子设计, 2017.01-2020.12, 63万元;

[8] 广东省自然科学基金, 面上项目, 基于高通量计算和人工智能的高效VOC捕获性能金属-有机骨架材料的自动设计, 2020.01-2023.12, 10万元;

[7] 广州大学百人计划, 科研启动项目, 高通量化工材料的设计、计算与合成, 2018.05-2023.05, 300万元;

[6] 广东省自然科学基金, 博士启动项目, 10万元;

[5] 中国博士后科学基金, 特别资助, 15万元;

[4] 中国博士后科学基金, 面上项目, 一等资助, 8万元;

[3] 华南理工大学中央高校项目, 面上项目, 8万元;

[2] 华南理工大学中央高校项目, 博士启动项目, 5万元;

[1] 华南理工大学制浆造纸工程国家重点实验室开放基金, 2万元。

**教学改革与质量工程等项目:**

2019国家级虚拟仿真实验教学项目——《香料紫罗兰酮合成工艺虚拟仿真实验》项目, 团队主要成员 (5/5)

2019年广东省高等教育教学成果二等奖, “虚、实”有机融合的化工类专业实践教学人才培养模式的创新与实践, 成果完成人 (6/8)

2019年广东省教育“双融双创”教师教育教学信息化交流及新媒体新技术教学应用三等奖, 成果完成人 (3/3)

2019年广州市教育教学信息化创新应用, 高教组二等奖, 成果完成人 (3/3)

**主要学术任职**

[1] 《Advances in Polymer Technology》客座主编。(SCI化工类Q2期刊, IF= 2.663)

[2] 中国化工学会化工新材料委员会会员;

[3] 广东省材料研究学会会员;

[4] 国家自然科学基金化学部函审专家;

**论文一览:**

发表科技/教学论文48篇, 其中SCI论文46篇, JCR Q1区论文35篇;

IF > 10论文10篇; IF > 7论文19篇; IF > 3论文34篇。

**27篇第一作者或通讯作者论文:**

(27) Zenan Shi, Hong Liang, Wenyuan Yang, Jie Liu, Zili Liu, Zhiwei Qiao\*, Machine learning and in silico discovery of metal-organic frameworks: Methanol as a working fluid in adsorption-driven heat pumps and chillers, Chemical Engineering Science, 2020, DOI: doi.org/10.1016/j.ces.2019.115430. (IF= 3.372, Q1区, top期刊, 化工三大期刊)

(26) Yongwei Chen, Houxiao Wu, Yinuo Yuan, Daofei Lv, Zhiwei Qiao\*, Dongli An, Xuanjun Wu, Hong Liang, Zhong Li, Qibin Xia\*, Highly rapid mechanochemical synthesis of a pillar-layer metal-organic framework for efficient CH<sub>4</sub>/N<sub>2</sub> separation, Chemical Engineering Journal, 2020, DOI: doi.org/10.1016/j.cej.2019.123836. (IF= 8.355, Q1区, top期刊)

(25) Xiaomei Deng, Wenyuan Yang, Shuhua Li, Hong Liang\*, Zenan Shi\*, Zhiwei Qiao\*, Large-scale screening and machine learning to predict the computation-ready, experimental metal-organic frameworks for CO<sub>2</sub> capture from air, Applied Sciences, 2020, 10, 569. (IF= 2.217, Q2区)

- (24) JieTao Hu, Jing Lin\*, Yayu Zhang, Zekai Lin, Zhiwei Qiao\*, Zili Liu, Wei Yang, Xiaoguo Liu, Mengyao Dong, Zhanhu Guo\*, A new anti-biofilm strategy of enabling arbitrary surfaces of materials and devices with robust bacterial anti-adhesion via spraying modified microspheres method, *Journal of Materials Chemistry A*, 2019, 7, 26039-26052. (IF= 10.733, Q1区, top期刊)
- (23) Hong Liang, Wenyuan Yang, Feng Peng, Zili Liu, Jie Liu, Zhiwei Qiao\*, Combining Large-Scale Screening and Machine Learning to Predict the Metal-Organic Frameworks for Organosulfurs Removal from High-Sour Natural Gas, *APL Materials*, 2019, 7, 091101. (IF= 4.296, top期刊)
- (22) Houxiao Wu, Yongwei Chen, Wenyuan Yang, Daofei Lv, Yinuo Yuan, Zhiwei Qiao\*, Hong Liang, Zhong Li, Qibin Xia\*, Ethane-selective behavior achieved on a nickel-based MOF: Impact of pore effect and hydrogen bonds, *Industrial & Engineering Chemistry Research*, 2019, 58, 10516. (IF= 3.375, Q1区, top期刊, 化工三大期刊)
- (21) Jinqiao Dong, Zhiwei Qiao (共同一作), Yutong Pan, Shing Bo Peh, Yi Di Yuan, Yuxiang Wang, Linzhi Zhai, Hongye Yuan, Youdong Cheng, Hong Liang, Bin Liu\*, and Dan Zhao\*, Encapsulation and Protection of Ultrathin Two-Dimensional Porous Organic Nanosheets within Biocompatible Metal-Organic Frameworks for Live-Cell Imaging, *Chemistry of Materials*, 2019, 31, 4897-4912. (IF= 10.159, Q1区, top期刊)
- (20) Long Liu, Zhiwei Qiao (共同一作), Xinfang Cui, Chunjiao Pang, Hong Liang, Peng Xie, Xuan Luo, Zuqiang Huang, Yanjuan Zhang, Zhongxing Zhao\*. Amino Acids Imprinted UiO-66s for Highly Recognized Adsorption of Small Angiotensin-Converting-Enzyme-Inhibitory Peptides, *ACS applied materials & interfaces*, 2019, 11, 23039-23049. (IF= 8.456, Q1区, top期刊)
- (19) Wenyuan Yang, Hong Liang, Feng Peng, Zili Liu, Jie Liu, Zhiwei Qiao\*, Computational screening of metal-organic framework membranes for the separation of 15 gas mixtures, *Nanomaterials*, 2019, 9: 467. (IF= 4.034, Q1区)
- (18) Zhiwei Qiao, Anthony K. Cheetham, Jianwen Jiang\*, Identifying the best metal-organic frameworks and unravelling different mechanisms for the separation of pentane isomers, *Molecular Systems Design & Engineering*, 2019, 4, 609. (IF= 2.708, Q2区)
- (17) Zhiwei Qiao, Qisong Xu, Jianwen Jiang\*, Computational screening of hydrophobic metal-organic frameworks for the separation of H<sub>2</sub>S and CO<sub>2</sub> from natural gas, *Journal of Materials Chemistry A*, 2018, 6, 18898. (IF= 10.733, Q1区, top期刊) (封面论文)
- (16) Zhiwei Qiao, Qisong Xu, Jianwen Jiang\*, High-throughput computational screening of metal-organic framework membranes for upgrading of natural gas, *Journal of Membrane Science*, 2018, 551: 47. (IF= 7.015, Q1区, top期刊)
- (15) Yongwei Chen, Zhiwei Qiao (共同一作), Jiali Huang, Houxiao Wu, Jing Xiao, Qibin Xia,\* Hongxia Xi, Jun Hu, Jian Zhou,\* Zhong Li. Unusual moisture-enhanced CO<sub>2</sub> capture within microporous PCN-250 frameworks, *ACS applied materials & interfaces*, 2018, 10, 38638. (IF= 8.456, Q1区, top期刊)

- (14) Yongwei Chen, Houxiao Wu, Daofei Lv, Wenyuan Yang, Zhiwei Qiao\*, Zhong Li, Qibin Xia\*, An ultramicroporous nickel-based metal-organic framework for adsorption separation of CO<sub>2</sub> over N<sub>2</sub> or CH<sub>4</sub>. *Energy & Fuels*, 2018, 32 (8), 8676. (IF= 3.021, Q2区)
- (13) 杨文远,梁红,乔智威\*.高通量筛选金属-有机框架: 分离天然气中的硫化氢和二氧化碳. *化学学报*, 2018, 76, 785. (IF= 2.463, Q2区)
- (12) Zhiwei Qiao, Qisong Xu, Anthony K. Cheetham, Jianwen Jiang\*. High-throughput computational screening of metal-organic frameworks for thiol capture; *Journal of Physical Chemistry C*, 2017, 121: 22208. (IF= 4.309, Q1区, top期刊)
- (11) Yongwei Chen, Zhiwei Qiao (共同一作), Daofei Lv, Houxiao Wu, Renfeng Shi, Qibin Xia\*, Haihui Wang, Jian Zhou\*, Zhong Li, Selective adsorption of light alkanes on a highly robust indium based metal-organic framework, *Industrial & Engineering Chemistry Research*, 2017, 56: 4488. (IF= 3.375, Q1区, top期刊, 化工三大期刊)
- (10) Zhiwei Qiao, Chunwang Peng, Jian Zhou, Jianwen Jiang\*, High-throughput computational screening of 137953 metal-organic frameworks for membrane separation of CO<sub>2</sub>/N<sub>2</sub>/CH<sub>4</sub> mixture, *Journal of Materials Chemistry A*, 2016, 4: 15904. (IF= 10.733, Q1区, top期刊) (封面论文)
- (9) Zhiwei Qiao, Kang Zhang, Jianwen Jiang\*, In silico screening of 4764 computation-ready, experimental metal-organic frameworks for CO<sub>2</sub> separation, *Journal of Materials Chemistry A*, 2016, 4(6): 2105. (IF= 10.733, Q1区, top期刊) (封面论文)
- (8) Zhiwei Qiao, Nanyi Wang, Jianwen Jiang, Jian Zhou\*, Design of amine functionalized metal-organic frameworks for CO<sub>2</sub> separation: the more amine, the better?, *Chemical Communications*, 2016, 52(5): 974. (IF= 6.164, Q1区, top期刊)
- (7) Zhiwei Qiao, Ariana Torres-Knoop, David Dubbeldam, David Fairen Jimenez, Jian Zhou\*, Randall Q. Snurr\*, Advanced Monte Carlo simulations of the adsorption of chiral alcohols in a homochiral metal-organic framework, *AIChE Journal*, 2014, 60(6): 2324. (IF= 3.463, Q1区, top期刊, 化工三大期刊)
- (6) Zhiwei Qiao, Jian Zhou\*, Xiaohua Lu, Designing new amine functionalized metal-organic frameworks for carbon dioxide/methane separation, *Fluid Phase Equilibria*, 2014, 362(1): 342. (IF= 2.514, Q1区)
- (5) Zhiwei Qiao, Haijun Feng, Jian Zhou\*, Molecular dynamics simulations on the melting of gold nanoparticles, *Phase Transitions*, 2014, 87 (1): 59. (SCI)
- (4) 乔智威, 李理波, 周健\*, 生物相容性金属-有机骨架材料负载药物的分子模拟研究, *高等学校化学学报*, 2014, 35 (12) : 2638. (SCI, 封面论文)
- (3) 乔智威, 杨仁党, 王海辉, 周健\*, 面向生物甲烷分离的不同金属配位金属-有机骨架材料的分子设计, *化工学报*, 2014, 65 (5) : 1729. (EI)
- (2) 乔智威, 任树化, 周健\*, H<sub>2</sub>S/N<sub>2</sub>混合物在碳纳米管中吸附分离的分子模拟, *高等学校化学学报*, 2012, 33 (4) : 800. (SCI)

(1) Zhiwei Qiao, Yili Wu, Xiaowei Li, Jian Zhou\*, Molecular simulation on the separation of water/ethanol azeotropic mixture by poly(vinyl alcohol) membrane, *Fluid Phase Equilibria*, 2011, 302: 14. (IF= 2.514, Q1区)

### 非第一作者/通讯作者文章:

(20) Jinqiao Dong, Yutong Pan, Heng Wang, Kuiwei Yang, Lingmei Liu, Zhiwei Qiao, Yi Di Yuan, Shing Bo Peh, Jian Zhang, Leilei Shi, Hong Liang, Yu Han, Xiaopeng Li, Jianwen Jiang, Bin Liu\*, Dan Zhao\*, Self-Assembly of Highly Stable Zirconium (IV) Coordination Cages with Aggregation Induced Emission (AIE) Molecular Rotors for Live-Cell Imaging, *Angewandte Chemie International Edition*, 2020, DOI: doi.org/10.1002/anie.201915199. (IF= 12.257, Q1区, top期刊)

(19) Libo Li, Yifan Duan, Shouwei Liao, Qia Ke, Zhiwei Qiao, Yanying Wei. Adsorption and separation of propane/propylene on various ZIF-8 polymorphs: Insights from GCMC simulations and the ideal adsorbed solution theory (IAST), *Chemical Engineering Journal*, 2020, DOI: doi.org/10.1016/j.cej.2019.123945. (IF= 8.355, Q1区, top期刊)

(18) Samraj Mollick, Soumya Mukherjee, Dongwook Kim, Zhiwei Qiao, Aamod V. Desai, Rajat Saha, Yogeshwar D. More, Jianwen Jiang, Myoung Soo Lah, Sujit K. Ghosh\*, Hydrophobic Shielding of Outer Surface: Enhancing the Chemical Stability of Metal–Organic Polyhedra, *Angewandte Chemie International Edition*, 2019, 58, 1041. (IF= 12.257, Q1区, top期刊)

(17) Wan Wei, Kang Zhang, Zhiwei Qiao, Jianwen Jiang\*, Functional UiO-66 for the removal of sulfur-containing compounds in gas and liquid mixtures: a molecular simulation study, *Chemical Engineering Journal*, 2019, 356, 737. (IF= 8.355, Q1区, top期刊)

(16) Yuhang Li, Zhiwei Qiao, Yonghai Cao, Hongjuan Wang, Hong Liang, Hao Yu, Feng Peng\*, Pathways of Superoxide Decay in Oxygen Reduction Reaction on Carbon-based Catalysts Evidenced by Theoretical Calculations, *ChemSusChem* 2019, 12(6): 1133. (IF= 7.804, Q1区, top期刊) (封面文章)

(15) Wanqing Li, Hongquan Fu, Yonghai Cao, Hongjuan Wang, Hao Yu, Zhiwei Qiao, Hong Liang, Feng Peng\*, Mn<sub>3</sub>O<sub>4</sub>@C Nanoparticles Supported on Porous Carbon as Bifunctional Oxygen Electrodes and their Electrocatalytic Mechanism, *ChemElectroChem*, 2019, 6(2): 359. (IF= 3.975, Q2区)

(14) Yuanyuan Shi, Zhiwei Qiao, Zili Liu\*, Jianliang Zuo, Cerium Doped Pt/TiO<sub>2</sub> for Catalytic Oxidation of Low Concentration Formaldehyde at Room Temperature, *Catalysis Letters*, 2019, 149 (5), 1319-1325. (IF= 2.372, Q2区)

(13) 魏炜,牟一蒙,梁红\*,李树华,乔智威,彭峰\*.不同金属负载对Cr/Al<sub>2</sub>O<sub>3</sub>-TiO<sub>2</sub>催化剂结构及氧化NO性能的影响.无机化学学报, 2019, 35, 978-986. (SCI)

- (12) Jingjing Jiao, Zijian Li, Zhiwei Qiao, Xu Li, Yan Liu\*, Jinqiao Dong, Jianwen Jiang\*, Yong Cui\*. Design and self-assembly of hexahedral coordination cages for cascade reactions, *Nature Communications*, 2018, 9, 4423. (IF= 11.878, Q1区, top期刊, Nature子刊)
- (11) Libo Li, Tao Zhang, Yifan Duan, Yanying Wei, Chaojie Dong, Li Ding, Zhiwei Qiao, Haihui Wang\*, Selective gas diffusion in two-dimensional MXene lamellar membranes: insights from molecular dynamics simulations, *Journal of Materials Chemistry A*, 2018, 6, 11734. (IF= 10.733, Q1区, top期刊) (hot paper)
- (10) Huang Chen, Libo Li\*, Tao Zhang, Zhiwei Qiao, Jinhui Tang, Jian Zhou\*, Protein Translocation through a MoS<sub>2</sub> Nanopore: A Molecular Dynamics Study, *Journal of Physical Chemistry C*, 2018, 122, 2070. (IF= 4.309, Q1区, top期刊)
- (9) Mark J. Purdue\*, Zhiwei Qiao, Molecular simulation study of wet flue gas adsorption on zeolite 13X, *Microporous and Mesoporous Materials*, 2018, 261: 181. (IF= 4.182, Q1区)
- (8) Yongwei Chen, Zhiwei Qiao, Houxiao Wu, Daofei Lv, Renfeng Shi, Qibin Xia\*, Jian Zhou\*, Zhong Li. An ethane-trapping MOF PCN-250 for highly selective adsorption of ethane over ethylene, *Chemical Engineering Science*, 2018, 175: 110. (IF= 3.372, Q1区, 化工三大期刊) (ESI高被引论文)
- (7) Yongwei Chen, Zhiwei Qiao, Daofei Lv, Chongxiong Duan, Xuejiao Sun, Houxiao Wu, Renfeng Shi, Qibin Xia\*, Zhong Li, Efficient adsorptive separation of C<sub>3</sub>H<sub>6</sub> over C<sub>3</sub>H<sub>8</sub> on flexible and thermoresponsive CPL-1, *Chemical Engineering Journal*, 2017, 328: 360. (IF= 8.355, Q1区, top期刊)
- (6) Jing Lin\*, Wei Wang, Wenli Bai, Mingning Zhu, Cheng Zheng, Zili Liu, Xianfang Cai, Dongdong Lu, Zhiwei Qiao, Fuqun Chen, Jiexing Chen, A gemini-type superspreader: Synthesis, spreading behavior and superspreading mechanism, *Chemical Engineering Journal*, 2017, 315: 262. (IF= 8.355, Q1区, top期刊)
- (5) Kang Zhang, Zhiwei Qiao, Jianwen Jiang\*, Molecular Design of Zirconium Tetrazolate Metal–Organic Frameworks for CO<sub>2</sub> Capture, *Crystal Growth & Design*, 2017, 17: 543. (IF= 4.153, Q1区, top期刊)
- (4) Krishna M Gupta, Zhiwei Qiao, Kang Zhang, Jianwen Jiang\*, Seawater Pervaporation through zeolitic imidazolate framework membranes: atomistic simulation study, *ACS applied materials & interfaces*, 2016, 8(21): 13392. (IF= 8.456, Q1区, top期刊)
- (3) 李映图, 乔智威, 李理波, 周健\*, *Materials Studio软件在分子模拟课程教学中的应用*, *广州化工*, 2016, 44 (21) : 160.
- (2) Nanyi Wang\*, Yi Liu, Zhiwei Qiao, Lisa Diestel, Jian Zhou, Aisheng Huang\*, Jürgen Caro, Polydopamine-based synthesis of a zeolite imidazolate framework ZIF-100 membrane with high H<sub>2</sub>/CO<sub>2</sub> selectivity, *Journal of Materials Chemistry A*, 2015, 3(8): 4722. (IF= 10.733, Q1区, top期刊)

(1) Zeric Hulvey, Keith V. Lawler, Zhiwei Qiao, Jian Zhou, David Fairen Jimenez, Randall Q. Snurr, Sergey V. Ushakov, Craig M. Brown, Paul M. Forster\*, Noble gas adsorption in copper trimesate, HKUST-1: an experimental and computational study, Journal of Physical Chemistry C, 2013, 117(39): 20116. (IF= 4.309, Q1区, top期刊) (ESI高被引论文)

**主要专利:**

[1] 彭峰, 周威, 谢谦, 乔智威, 李俊杰, 曹正伟.一种用于纳米碳酸钙表面改性的连续反应砂磨装置, ZL201821194095.5, 2019年授权

[2] 彭峰, 刘运鹏, 梁红, 乔智威.一种具有高光催化活性的还原二氧化钛制备方法, ZL201810235381.X, 2018

上一篇: 汪黎明个人简介

下一篇: 党成雄个人简介

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