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## 施慧



1983年1月29日生, 汉族, 江苏常熟人

研究领域: 物理化学, 多相催化, 化学动力学

主要研究方向: 能源催化转化反应中物理化学原理, 多相催化剂的理性设计与创制, 过程强化的创新工艺

ResearcherID: <http://www.researcherid.com/rid/J-7083-2014>

Citations: 900 (截至2018年2月底, Google Scholar数据)

<http://scholar.google.com/citations?user=oxqHT-oAAAAJ>

## 教育背景

1. 2008-2012: 博士, 工业化学系 (化学、化学反应工程), 慕尼黑工业大学, 德国 (导师: Johannes A. Lercher教授)

“Structural requirements and reaction pathways of hydrogenolytic C-C bond cleavage in naphthenes over supported platinum and iridium domains” (负载型铂和铱催化剂上环烷烃氢解反应的结构敏感性及机理) (荣誉: Summa Cum Laude, 最优等博士论文)

2. 2001-2008: 本科 (化学) 及硕士 (物理化学), 清华大学 (导师: 徐柏庆教授)

负载型金催化剂上  $\alpha,\beta$ -不饱和醛的选择加氢反应 (“Chemoselective hydrogenation of  $\alpha,\beta$ -unsaturated aldehydes on supported gold catalysts”)

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## 研究经历和主要学术贡献 ( 参见 Research Profile and Highlights )

1. 2017.6至今 高级研究助手, 慕尼黑工业大学 (TUM):

<https://www.tc2.ch.tum.de/index.php?id=2940> (Co-PI)

- 主持工业合作研究项目“负载及非负载型过渡金属硫化物的催化反应”: 多环芳烃深度加氢、杂环芳烃脱硫脱氮 ( 美国 Chevron 公司资助 )

2. 2013.3-2017.5 博士后, 美国西北太平洋国家实验室 (PNNL):

- 生物质( 模型分子及真实原料 )催化转化为化学品和能源过程中的动力学和反应机理( 美国能源部基础能源科学项目资助, 研究对象及反应类型涵盖: 金属催化的芳醚、烷芳醚水解或醇解反应; 限域空间内水合质子的结构及形成机制; 酸催化醇类脱水及碳碳偶联反应 ( 气相和不同液相溶剂 ), 首创性地研究了一种特殊的主客体多相限域催化体系, 即分子尺寸级别的酸性分子筛孔道内的水合质子, 揭示了其酸催化的活性规律及物理化学内因
- 结合原位谱学、反应动力学及理论计算等手段深入理解决定多相催化剂 ( 负载型金属及多孔酸性材料 ) 在水相和其他液相反应中活性、选择性和稳定性的物理化学及微观结构因素, 并在此前提下设计高效且稳定的催化材料用于生物质转化及其他凝聚相反应过程
- 采用特定检测界面-表面化学物种的和频振动光谱 (SFG-VS)原位观测液相催化、电催化及相关 ( 如吸附 ) 过程
- 二氧化碳催化转化项目, 提出负载型钨、钨催化剂上二氧化碳催化还原为一氧化碳和甲烷的反应中表面活性位、中间体及选择性的关联

3. 2008.9-2012.12, 博士, 慕尼黑工业大学:

- 提出金属纳米颗粒催化的烷烃氢解及环烷烃开环反应的活性位本质、反应机理, 首次建

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立此类气相催化反应清晰严谨的结构-性能关系

- 研究固体酸碱材料和金属-固体酸双功能催化剂上多种反应 ( 烷烃裂解 , 氢转移 , 烷基化 ) 的结构-性能关系 , 为创制新型催化材料提供明确指导
- 结合同位素标记实验和统计热力学计算证明贵金属表面烷烃氢解反应机理
- 参与甲醇制丙烯(MTP)过程的系统研究 , 提出共进料对基于芳烃、烯烃的催化循环的动力学影响并首次发现与催化剂失活有关的一条新的氢转移路径
- 设计并构建了应用于多相催化剂筛选的多通道反应系统与数据采集和分析系统

4. 2004-2008 , 硕士 , 清华大学:

- 负载型纳米金颗粒催化的 1,3-丁二烯及共轭不饱和醛酮选择加氢反应 , 发现表面高度分散的氧化态金物种是高活性、高选择性及高稳定性丁二烯选择加氢催化的关键因素
- 设计和制备可控尺寸的胶体金纳米颗粒及高比表面氧化物 , 研究液相共轭不饱和醛酮选择加氢反应中的尺寸效应

## 教学

2008-2011: 工业化学实验课(“Technische Chemie Praktikum”, 慕尼黑工业大学)

2005-2006: 催化化学 ( 研究生课程 ) 助教 ( 清华 )

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## 学术兼职、荣誉及获奖情况

- 2017起担任学术期刊 ChemCatChem的顾问编委 ( International Advisory Board ) :  
([http://onlinelibrary.wiley.com/journal/10.1002/\(ISSN\)1867-3899/homepage/2491\\_edbd.html](http://onlinelibrary.wiley.com/journal/10.1002/(ISSN)1867-3899/homepage/2491_edbd.html))
- 2016年7月至2017年5月共同主持西北太平洋国家实验室的化学转化重大项目 ( Chemical Transformation Initiative ) 中的酸碱催化子课题 ( Co-PI for Thrust 2: Acid-Base Catalysis for Converting ECH Intermediates )
- 2014年荣获美国西北太平洋国家实验室的杰出表现奖 ( Outstanding Performance Award )
- 2015至今 , American Chemical Society (ACS) 会员
- 为十数种主流催化及顶级化学期刊担任审稿人,主要杂志包括Angewandte Chemie (授予2016年most outstanding referee, 排名前5%), Journal of Catalysis, ChemSusChem, ChemCatChem, Journal of Materials Chemistry A, Catalysis Science and Technology等。被Elsevier和Wiley出版社评为杰出审稿人 ( Outstanding Reviewer )

## 译著

于2007-2008年参与翻译“Catalysis by Gold” (作者 : Geoffrey C. Bond, Catherine Louis and David T. Thompson, Imperial College Press) (中文版 : 《黄金的催化作用 : 现象 , 原理与应用 , 科学出版社》 )

## 论文

已发表论文 31 篇，包括一作及通讯作者文章 10 篇，第二作者文章 13 篇

### 通讯作者文章

- 1) Y. Liu, E. Barath, H. Shi\*, J. Hu, D.M. Camaioni, J.A. Lercher\*. Solvent-determined mechanistic pathways in zeolite-H-BEA-catalysed phenol alkylation. *Nature Catalysis*, 1 (2018) 141-147.
- 2) K.A. Resende, C.E. Hori\*, F.B. Noronha, H. Shi\*, O.Y. Gutierrez, D.M. Camaioni, J.A. Lercher. Aqueous phase hydrogenation of phenol catalyzed by Pd and PdAg on ZrO<sub>2</sub>. *Applied Catalysis A: General*, 548 (2017) 128-135.

### 第一作者文章

- 1) Z. Zhao,<sup>†</sup> H. Shi,<sup>†</sup> C. Wan, M.Y. Hu, Y. Liu, D. Mei, D.M. Camaioni, J.Z. Hu\*, J.A. Lercher\*. Mechanism of Phenol Alkylation in Zeolite H-BEA Using In Situ Solid-State NMR Spectroscopy. *Journal of the American Chemical Society*, 139 (2017) 9178–9185 (†: equal contribution).
- 2) **H. Shi**, S. Eckstein, A. Vjunov, D.M. Camaioni, J.A. Lercher\*. Tailoring nanoscopic confines to maximize catalytic activity of hydronium ions. *Nature Communications*, 8 (2017) 15442.
- 3) **H. Shi**, X.-Y. Yu\*, J.A. Lercher. Sailing into uncharted waters: recent advances in the in situ monitoring of catalytic processes in aqueous environments (**Front Cover**), *Catalysis Science and Technology*, 5 (2015) 3035–3060.
- 4) **H. Shi**, O.Y. Gutiérrez\*, A. Zheng, G.L. Haller, J.A. Lercher\*. Mechanistic pathways for methylcyclohexane hydrogenolysis over supported Ir catalysts, *Journal of Physical Chemistry C*, 118 (2014) 20948–20958.
- 5) **H. Shi**, O.Y. Gutiérrez, H. Yang, N.D. Browning, G.L. Haller, J.A. Lercher\*. Catalytic consequences of particle size and chloride promotion in the ring opening of cyclopentane on Pt/Al<sub>2</sub>O<sub>3</sub>, *ACS Catalysis*, 3 (2013) 328–338.

- 6) H. Shi, O.Y. Gutiérrez, G.L. Haller, D. Mei, R. Rousseau, J.A. Lercher\*. Structure sensitivity of hydrogenolytic cleavage of endocyclic and exocyclic C–C bonds in methylcyclohexane over supported iridium particles, *Journal of Catalysis*, 297 (2013) 70–78.
- 7) H. Shi, X. Li, G.L. Haller, O.Y. Gutiérrez, J.A. Lercher\*. Active sites and reactive intermediates in the hydrogenolytic cleavage of C–C bonds in cyclohexane over supported iridium clusters, *Journal of Catalysis*, 295 (2012) 133–145.
- 8) H. Shi, N. Xu, D. Zhao, B.-Q. Xu\*. Immobilized PVA-stabilized gold nanoparticles on silica show an unusual selectivity in the hydrogenation of cinnamaldehyde. *Catalysis Communications*, 9 (2008) 1949–1954.

#### 其他共同作者文章 (按年份排序)

- 1) A. Vjunov, M. Wang, N. Govind, T. Huthwelker, H. Shi, D. Mei\*, J.L. Fulton\*, J.A. Lercher\*. Tracking the chemical transformations at the Brønsted acid site upon water-induced deprotonation in a zeolite pore. *Chemistry of Materials*, 29 (2017) 9030–9042.
- 2) S. Proding, H. Shi, S. Eckstein, J.Z. Hu, M.V. Olarte, D.M. Camaioni, M.A. Derewinski\*, J.A. Lercher\*. Stability of Zeolites in Aqueous Phase Reactions. *Chemistry of Materials*, 29 (2017) 7255–7262.
- 3) X. Wang, H. Shi, J. Szanyi\*. Controlling selectivities in CO<sub>2</sub> reduction through mechanistic understanding. *Nature Communications*, 8 (2017) 513.
- 4) C. Song, Y. Chu, M. Wang, H. Shi, L. Zhao, X. Guo, W. Yang, J. Shen, N. Xue\*, L. Peng\*, W. Ding\*. Cooperativity of adjacent Brønsted acid sites in MFI zeolite channel leads to enhanced polarization and cracking of alkanes. *Journal of Catalysis*, 349 (2017) 163–174.
- 5) Y. Liu, A. Vjunov, H. Shi, S. Eckstein, D.M. Camaioni, D. Mei, E. Barath, J.A. Lercher\*. Enhancing the catalytic activity of hydronium ions through constrained environments. *Nature Communications*, 8 (2017) 14113.

- 6) M. Wang, **H. Shi**, D.M. Camaioni, J.A. Lercher\*. Palladium-Catalyzed Hydrolytic Cleavage of Aromatic C-O Bonds (**Hot paper**), *Angewandte Chemie International Edition*, 56 (2017) 2110–2114.
- 7) Y. Zhi, **H. Shi**, L. Mu, Y. Liu, D. Mei, D.M. Camaioni, J.A. Lercher\*. Dehydration pathways of 1-propanol on HZSM-5 in the presence and absence of water. *Journal of the American Chemical Society*, 137 (2015) 15781–15794.
- 8) S. Kasakov, **H. Shi**, D.M. Camaioni, C. Zhao, E. Barath\*, A. Jentys, J.A. Lercher\*. Reductive deconstruction of organosolv lignin catalyzed by zeolite supported nickel nanoparticles, *Green Chemistry*, 17 (2015) 5079–5090.
- 9) X. Wang, **H. Shi**, J.H. Kwak, J. Szanyi\*. Mechanism of CO<sub>2</sub> hydrogenation on Pd/Al<sub>2</sub>O<sub>3</sub> catalysts: kinetics and transient DRIFTS-MS studies, *ACS Catalysis*, 5 (2015) 6337–6349.
- 10) Z. A. Chase, S. Kasakov, **H. Shi**, A. Vjunov, J. L. Fulton\*, D. M. Camaioni\*, M. Balasubramanian, C. Zhao, Y. Wang, J. A. Lercher\*. State of Supported Nickel Nanoparticles during Catalysis in Aqueous Media. *Chemistry-A European Journal*, 21 (2015) 16541–16546.
- 11) X. Wang, Y.C. Hong, **H. Shi**, J. Szanyi\*. Kinetic modeling and transient DRIFTS-MS studies of CO<sub>2</sub> methanation over Ru/Al<sub>2</sub>O<sub>3</sub> catalysts. *Journal of Catalysis*, 343 (2016) 185–195.
- 12) S. Kasakov, C. Zhao, E. Barath, Z.A. Chase, J.L. Fulton, D.M. Camaioni, A. Vjunov, **H. Shi**, J.A. Lercher\*. Glucose- and Cellulose-Derived Ni/C-SO<sub>3</sub>H Catalysts for Liquid Phase Phenol Hydrodeoxygenation, *Chemistry-A European Journal*, 21 (2015) 1567–1577.
- 13) J.Z. Hu\*, M.Y. Hu, Z.C. Zhao, S.C. Xu, A. Vjunov, **H. Shi**, D.M. Camaioni, C.H.F. Peden, J.A. Lercher. Sealed rotors for *in situ* high temperature high pressure MAS NMR, *Chemical Communications*, 51 (2015) 13458–13461.
- 14) X. Sun, S. Mueller, **H. Shi**, G.L. Haller, M. Sanchez-Sanchez, A.C. van Veen, J.A. Lercher\*. On the impact of co-feeding aromatics and olefins for the methanol-to-olefins reaction on HZSM-5, *Journal of Catalysis*, 314 (2014) 21–31.
- 15) X. Sun, S. Mueller, Y. Liu, **H. Shi**, G. L. Haller, M. Sanchez-Sanchez, A. C. van Veen, J. A. Lercher\*. On reaction pathways in the conversion of methanol to hydrocarbons on HZSM-5, *Journal of Catalysis*, 317 (2014) 185–197.

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- 16) F. Schuessler, S. Schallmoser, **H. Shi**, G.L. Haller, E.E. Ember, J.A. Lercher\*. Enhancement of dehydrogenation and hydride transfer by  $\text{La}^{3+}$  cations in zeolites during acid catalyzed alkane reactions, *ACS Catalysis*, 4 (2014) 1743–1752.
- 17) S. Scholz, **H. Shi**, J. A. Lercher\*. Controlled Synthesis of Platinum Loaded Hierarchic Silica Spheres, *Topics in Catalysis*, 55 (2012) 800.
- 18) X. Zhang, **H. Shi**, B.-Q. Xu\*. Vital roles of hydroxyl groups and gold oxidation states in Au/ZrO<sub>2</sub> catalysts for 1,3-butadiene hydrogenation, *Journal of Catalysis*, 279 (2011) 75–87.
- 19) D.-P. He, **H. Shi**, Y. Wu, B.-Q. Xu\*. Synthesis of chloroanilines: selective hydrogenation of the nitro in chloronitrobenzenes over zirconia-supported gold catalyst. *Green Chemistry*, 9 (2007) 849–851.
- 20) X. Zhang, **H. Shi**, B.-Q. Xu\*. Comparative study of Au/ZrO<sub>2</sub> catalysts in CO oxidation and 1,3-butadiene hydrogenation. *Catalysis Today*, 122 (2007) 330–337.
- 21) X. Zhang, **H. Shi**, B.-Q. Xu\*. Catalysis by gold: Isolated surface Au<sup>3+</sup> ions are active sites for selective hydrogenation of 1,3-butadiene over Au/ZrO<sub>2</sub> catalysts. *Angewandte Chemie International Edition*, 44 (2005) 7132–7135.

## 会议口头报告及墙报

\*本人为报告人

- 1) **H. Shi\***, Y. Liu, D.M. Camaioni, J.A. Lercher, “Kinetic and mechanistic roles of co-reactant and solvent in phenol alkylation on solid acids” (oral), 253rd ACS National Meeting, 2017, San Francisco, USA.
- 2) **H. Shi\***, D.M. Camaioni, J.A. Lercher, “Towards understanding acid-catalyzed alcohol dehydration in aqueous phase: Kinetics, mechanism and energetic landscapes” (oral), 251st ACS National Meeting, 2016, San Diego, USA.
- 3) **H. Shi\***, A. Vjunov, D.M. Camaioni, J.A. Lercher, “Solvent effects in biomass conversion on solid acids in liquid phase” (oral), 24<sup>th</sup> North American Meeting (NAM) of the Catalysis Society,



2015, Pittsburgh, USA.

4) **H. Shi\***, Stanislav Kasakov, Eszter Baráth, D.M. Camaioni, J.A. Lercher, "Reductive deconstruction of organosolv lignin catalyzed by zeolite supported Ni nanoparticles" (oral), Annual Meeting of the Pacific Coast Catalysis Society, 2015, Richland, USA.

5) **H. Shi\***, O.Y. Gutiérrez, J.A. Lercher, "On the apparent and intrinsic structure sensitivities of hydrogenolytic C-C bond cleavages of C<sub>6</sub>-naphthenics over supported Ir clusters" (poster). 15th International Congress on Catalysis, 2012, Munich, Germany.

6) **H. Shi\***, O.Y. Gutiérrez, J.A. Lercher, "Structural requirements of direct ring opening of cyclohexane over supported Ir clusters" (poster). 45. Jahrestreffen Deutscher Katalytiker, 2012, Weimar, Germany.

7) **H. Shi\***, O.Y. Gutiérrez, J.A. Lercher, "A detailed kinetic study of the direct ring opening of cyclohexane and methylcyclohexane over monofunctional Ir/Al<sub>2</sub>O<sub>3</sub> catalysts" (poster). Deutsche Wissenschaftliche Gesellschaft (DGfMK) Annual Conference, 2011, Dresden, Germany.

8) H. Shi, Y. Liu, J.Z. Hu, D.M. Camaioni, J.A. Lercher, "Solid-Acid-Catalyzed Alkylation of Phenol in Aqueous and Hydrocarbon Solvents" (oral), 25th North American Meeting (NAM) of the Catalysis Society, 2017, Denver, USA.

9) W. Luo, E. Schachtl, H. Shi, O.Y. Gutiérrez, J.A. Lercher, "Understanding the High Activity of Ni-Promoted WS<sub>2</sub> for Hydrogenation of Polyaromatic Compounds" (oral), 25th North American Meeting (NAM) of the Catalysis Society, 2017, Denver, USA.

10) S. Albersberger, M. Wagenhofer, O.Y. Gutiérrez, H. Shi, J.A. Lercher, "Hydrogenation and C-N Bond Cleavage of Aromatic Compounds on Ni-Mo-W Sulfides" (oral), 25th North American Meeting (NAM) of the Catalysis Society, 2017, Denver, USA.

11) J.Z. Hu, H. Shi, M. Hu, C. Wan, M. Wang, Z. Zhao, N. Jaegers, S. Proding, M. Derewinski, A. Vjunov, D.M. Camaioni, C.H.F. Peden, Y. Wang, J.A. Lercher, "Operando Magic Angle Spinning NMR Spectroscopy for Catalysis" (oral), 25th North American Meeting (NAM) of the Catalysis Society, 2017, Denver, USA.

12) M. Wang, H. Shi, D.M. Camaioni, J.A. Lercher, "Palladium Catalyzed Aromatic C-O Bond

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Cleavage of Aryl Ethers" (oral), 25th North American Meeting (NAM) of the Catalysis Society, 2017, Denver, USA.

13) Z. Chase, H. Shi, D.M. Camaioni, J. Fulton, M. Balasubramanian, Y. Wang, J.A. Lercher, "On the Local Structure and Catalytic Performance of a NiFe Bimetallic Catalyst for Aqueous Phase Phenol Hydrogenation" (poster), 25th North American Meeting (NAM) of the Catalysis Society, 2017, Denver, USA.

14) X. Wang, **H. Shi**, D. Ferri, J. Szanyi, "Does particle size affect the mechanism of CO<sub>2</sub> hydrogenation on Pd/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub> catalysts? A combined kinetics/DRIFTS/ME-FTIR/MS study" (oral), 16th International Congress on Catalysis, 2016, Beijing, China.

15) X. Wang, **H. Shi**, J. Szanyi, "The mechanism of CO<sub>2</sub> hydrogenation over Pd/Al<sub>2</sub>O<sub>3</sub>: a steady state isotopic transient kinetic analysis (SSITKA)/operando-FTIR spectroscopy investigation" (poster), 16th International Congress on Catalysis, 2016, Beijing, China.

16) Y. Zhi, **H. Shi**, D. Mei, J. A. Lercher, "Impact of water on dehydration of alcohols on molecular sieves" (oral), 251st ACS National Meeting, 2016, San Diego, USA.

17) S. Scholz, B.B. Molinos, **H. Shi**, J.A. Lercher, "Influence of surface modified mesoporous silica on the stability and reactivity of platinum nanoparticles" (poster). 43. Jahrestreffen Deutscher Katalytiker, 2010, Weimar, Germany.