

化工学院导师个人情况表

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个人简介

教育经历:

1997 年 9 月- 2001 年 7 月: 北京化工大学理学院应用数学专业 (学士学位)

2001 年 9 月- 2004 年 6 月: 北京化工大学化学工程学院化学工程专业 (硕士学位)

导师: 汪文川教授

2004 年 9 月- 2008 年 11 月: van't Hoff Institute for Molecular Sciences,  
University of Amsterdam (荷兰阿姆斯特丹大学,  
导师: Prof. Berend Smit) (博士学位)

工作经历:

2005 年 1 月- 2005 年 7 月: Centre Européen de Calcul Atomique et Moléculaire  
(CECAM) (欧洲原子/分子计算中心, 法国里昂)  
(visiting student)

2006 年 10 月- 2006 年 12 月: University Pablo de Olavide, Seville, Spain (西班牙塞  
维利亚 Dr. Sofia Calero 研究组)  
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2008 年 3 月- 2008 年 8 月: University of California, Berkeley (美国加州大学伯克利  
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2008年12月-2009年11月: University of California, Berkeley (美国加州大学伯克利分校) (博士后)

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### 发表论文

1. **Bei Liu**, Changyu Sun, and Guangjin Chen, Molecular simulation studies of separation of CH<sub>4</sub>/H<sub>2</sub> mixture in metal-organic frameworks with interpenetration and mixed-ligand, *Chem. Eng. Sci.* **2011**, *66*, 3012-3019.
2. **Bei Liu**, Xiulin Wang, Xulong Tang, Lanying Yang, Changyu Sun, and Guangjin Chen, Recovery of hydrogen from ammonia plant tail gas by absorption-hydration hybrid method, *Chin. J. Chem. Eng.* **2011**, in press.
3. **Bei Liu** and Berend Smit\*, Molecular simulation studies of separation of CO<sub>2</sub>/N<sub>2</sub>, CO<sub>2</sub>/CH<sub>4</sub>, and CH<sub>4</sub>/N<sub>2</sub> by ZIFs, *J. Phys. Chem. C* **2010**, *114*, 8515-8522.
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5. **Bei Liu**, Qingyuan Yang, Chunyu Xue, Chongli Zhong, and Berend Smit, Molecular simulation of hydrogen diffusion in interpenetrated metal-organic frameworks, *Phys. Chem. Chem. Phys.* **2008**, *10*, 3244-3249. (封面论文)
6. **Bei Liu**, Qingyuan Yang, Chunyu Xue, Chongli Zhong, Biaohua Chen, and Berend Smit, Enhanced adsorption selectivity of hydrogen/methane mixtures in metal-organic frameworks with interpenetration: A molecular simulation study, *J. Phys. Chem. C* **2008**, *112*, 9854-9860.
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10. **Bei Liu** and Berend Smit, Molecular simulation of adsorption of alkanes in sodium MOR-type zeolites using a new force field, *Phys. Chem. Chem. Phys.* **2006**, *8*, 1852-1857.
11. **Bei Liu**, Wenchuan Wang, and Xianren Zhang, A hybrid cylindrical model for characterization of MCM-41 by Density Functional Theory, *Phys. Chem. Chem. Phys.* **2004**, *6*, 3985-3990.
12. **刘蓓**, 张现仁, MCM-41中混合势模型及简单流体吸附的巨正则Monte Carlo模拟, 计算

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机与应用化学, **2004**, *21*, 685-689.

13. Dong Wu, Cuicui Wang, **Bei Liu**, Dahuan Liu, Qingyuan Yang, and Chongli Zhong, Large scale computational screening of metal-organic frameworks for CH<sub>4</sub>/H<sub>2</sub> separation, *AIChE J.* **2011**, in press.
14. Jun Chen, Changyu Sun, **Bei Liu**, Baozi Peng, Xiulin Wang, Guangjin Chen, Julian Y. Zuo, and Heng-Joo Ng, Metastable boundary conditions of water-in-oil emulsions in the hydrate formation region, *AIChE J.* **2011**, in press.
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18. Hongliang Huang, Wenjuan Zhang, Dahuan Liu, **Bei Liu**, Guangjin Chen, and Chongli Zhong, Effect of temperature on gas adsorption and separation in ZIF-8: A combined experimental and molecular simulation study, *Chem. Eng. Sci.* **2011**, *66*, 6297-6305.
19. N. E. R. Zimmermann, M. Haranczyk, M. Sharma, **Bei Liu**, B. Smit, and F. J. Keil, Adsorption and diffusion in zeolites: the pitfall of isotopic crystal structures, *Molecular Simulation* **2011**, *37*, 986 – 989.
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22. Qiang Sun, Xuqiang Guo, Aixian Liu, **Bei Liu**, Yusheng Huo, and Guangyin Chen, Experimental study on the separation of CH<sub>4</sub> and N<sub>2</sub> via hydrate formation in TBAB solution, *Ind. Eng. Chem. Res.* **2011**, *50*, 2284-2288.
23. Changyu Sun, Wenzhi Li, Xin Yang, Fengguang Li, Qing Yuan, Liang Mu, Jun Chen, **Bei Liu**, and Guangjin Chen, Progress in Research of Gas Hydrate, *Chin. J. Chem. Eng.* **2011**, *19*, 151-162. (**Invited Review**)
24. Qingyuan Yang, Qing Xu, **Bei Liu**, Chongli Zhong, and Berend Smit, Molecular simulation of CO<sub>2</sub>/H<sub>2</sub> mixture separation in metal-organic frameworks: Effect of catenation and electrostatic interactions, *Chin. J. Chem. Eng.* **2009**, *17*, 781-790.

25. Chunyu Xue, Zie Zhou, **Bei Liu**, Qingyuan Yang, and Chongli Zhong, Methane diffusion mechanism in catenated metal-organic frameworks, *Molecular Simulation* **2009**, *35*, 373-380.
26. Elena Garcia-Perez, David Dubbeldam, **Bei Liu**, Berend Smit, and Sofia Calero, A computational method to characterize framework aluminum in aluminosilicates, *Angew. Chem. Int. Ed.* **2007**, *46*, 276-278.
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28. 谢超然, **刘蓓**, 李长江, 杜恺, 黄维民, 李玉民, 硅酸铝纤维喷涂工艺在裂解炉中的应用, *乙烯工业*, **2002**, *14*, 39-42.
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### 科研项目

序号	项目、课题名称 (下达编号)	项目来源、属何种项目	本人可支配经费(万元)	是否负责人
1	生物金属-有机骨架材料中的复杂主客体作用研究 (21006126)	国家自然科学基金委员会 (国家自然科学基金青年基金)	20	是
2	金属-有机骨架材料和沸石用于天然气净化的分子模拟研究 (20100007120009)	教育部 (高等学校博士学科点专项科研基金)	3.6	是
3	金属-有机骨架材料和沸石用于天然气净化的分子模拟与实验研究 (BJBJRC-2010-01)	中国石油大学 (北京) (重点学科青年拔尖人才基金)	20	是

4	北京市科技新星人才专项基金 (2010B069)	北京市科学技术委员会	10	是
<b>获得奖励</b>				
<p><b>2011年</b>：北京市科技新星</p> <p><b>2010年</b>：中国石油大学（北京）校重点学科青年拔尖人才</p>				
<b>出版专著</b>				
<p>1. <b>Bei Liu</b>, Weixin Pang, Baozi Peng, Changyu Sun, and Guangjin Chen, Heat Transfer Related to Gas Hydrate Formation/Dissociation, 2011, pp. 477 - 502. One chapter for the book "<i>Developments in Heat Transfer</i>" (ISBN 978-953-307-569-3).</p>				
<b>获得专利</b>				
<b>其它</b>				