个人信息

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工作经历

2013.6 至今	杭州师范大学医学院药学系	校聘教授
2009.9-2013.6	Max Planck Institute for Polymer Research	Research Associate
	(马克斯-普朗克高分子研究所,德国)	研究助理

教育背景

2004.9-2009.6	浙江大学	化学系	化学博士	
2003.1-2003.6	香港大学	化学系	交换学生	
2000.9-2004.6	浙江大学	化学系	理学学士	

主要研究领域

- 药物传递及载药材料的分子模拟
- 生物分子表面吸附的分子模拟
- 多尺度模拟方法的发展
- 二维纳米材料的制备及计算机模拟

主持科研项目与人才计划

苏州高新区科技创新创业领军孵化人才、2015

国家自然科学基金青年项目、多肽与无机晶体相互作用的多尺度模拟方法研究、25万、负责人、2015.1-2017.12。

获奖及荣誉

2011.9	Best Poster Award, Max Planck Institute for Polymer Research Posterday 2011
2010.6	Biomaterials 期刊 2006-2010 中国大陆 top50 高引论文
2009-2010	Max Planck Society Research Fellow, Germany
2009.6	由中德科学中心选拔,代表中国博士生参加第59界德国林岛诺贝尔奖获得者大会
2007-2008	浙江大学优秀研究生二等荣誉
2007-2008	浙江大学光华奖学金

- L.J. Liang*, J.W. Shen*, Z.S. Zhang, Q. Wang*. DNA sequencing by two-dimensional materials: As theoretical modeling meets experiments. *Biosensors and Bioelectronics*, accepted. doi:10.1016/j.bios.2015.12.037.
- L.J. Liang, E.Y. Chen, J.W. Shen*, Q. Wang*. Molecular modeling of translocation of biomolecules in carbon nanotubes: method, mechanism and application. *Molecular Simulation*, accepted.
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- **J.W. Shen**, T. Tang, X.H. Wei, W. Zheng, T.Y. Sun, Z.S. Zhang, L.J. Liang*, Q. Wang*. On the loading mechanism of ssDNA into carbon nanotubes. *RSC Advances*, 2015, 5, 56896.
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- **J.W. Shen,** C.L. Li, N.F.A. van der Vegt, C. Peter. Understanding the control of mineralization by polyelectrolyte additives: simulation of preferential binding to calcite surfaces. *Journal of Physical Chemistry C* 2013, 117, 6904.
- C.L. Li, **J.W. Shen,** C. Peter, N.F.A. van der Vegt. A Chemically accurate implicit-solvent coarse-grained model for polystyrenesulfonate solutions. *Macromolecules* 2012, 45, 2551.
- **J.W. Shen,** C.L. Li, N.F.A. van der Vegt, C. Peter. Transferability of coarse grained potentials: implicit solvent models for hydrated ions. *Journal of Chemical Theory and Computation* 2011, 7, 1916.

- Y. Kang, Q. Wang, Y.C. Liu, **J.W. Shen**, T. Wu. Diameter selectivity of protein encapsulation in carbon nanotubes. *Journal of Physical Chemistry B* 2010, 114, 2869.
- **J.W. Shen**, T. Wu, Q. Wang, Y. Kang, X. Chen. Adsorption of insulin peptide on charged single-walled carbon nanotubes: significant role of ordered waters. *ChemPhysChem* 2009, 10, 1260.
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- L.J. Liang, Q. Wang, T. Wu, **J.W. Shen,** Y. Kang. Molecular dynamics simulation on stability of insulin on graphene. *Chinese Journal of Chemical Physics* 2009, 22, 627.
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- Y.C. Liu, **J.W. Shen**, K.E. Gubbins, J. D. Moore, T. Wu, Q. Wang. Diffusion dynamics of water controlled by topology of potential energy surface inside carbon nanotubes. *Physical Review B* 2008, 77, 125438. (featured in *Virtual Journal of Nanoscale Science & Technology*)
- **J.W. Shen**, T. Wu, Q. Wang, H.H. Pan. Molecular simulation of protein adsorption and desorption on hydroxyapatite surfaces. *Biomaterials* 2008, 29, 513. (**Leading Opinion Paper**, one of 12 figures featured in "2008 The Year in Images" of *Biomaterials*)
- **J.W. Shen**, T. Wu, Q. Wang, Y. Kang. Induced stepwise conformational change of human serum albumin on carbon nanotube surfaces. *Biomaterials* 2008, 29, 3847. (one of 12 figures featured in "2008 The Year in Images" of *Biomaterials*)
- X. Chen, T. Wu, Q. Wang, **J.W. Shen**. Shield effect of silicate on adsorption of protein onto silicon-doped hydroxyapatite (100) surface. *Biomaterials* 2008, 29, 2423.
- F. Liu, X.S. Ye, T. Wu, C.T. Wang, **J.W. Shen**, Y. Kang. Conformational mobility of GOx coenzyme complex on single-wall carbon nanotubes. *Sensors* 2008, 8, 8453.
- X. Chen, Q. Wang, **J.W. Shen**, H.H. Pan, T. Wu. Adsorption of leucine-rich amelogenin protein on hydroxyapatite (001) surface through –COO⁻ claws. *Journal of Physical Chemistry C* 2007, 111, 1284.
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- **J.W. Shen**, T. Wu, Y.G. Wang, Q. Wang. Quantum mechanics study on the selectivity of alkali metal cations by a novel fluorescent chemosensor. *Molecular Simulation* 2006, 32, 1123.

国际会议及报告

244th American Chemical Society National Meeting & Expositon

2012 年 8 月 19-23 日, Philadelphia, 美国 (会议报告)

SPP 1420 Winter School & International Conference for Bio-inspired Materials

2012年4月19-23日, Potsdam, 德国 (会议报告)

Perspectives and Challenges of Simulations at Bio-materials Interfaces

2011年10月10-14日, Bremen, 德国

Mainz Materials Simulation Days

2011年5月25-27日, Mainz, 德国

5th Rhein-Main-Modelling Meeting

2010年12月7日, Darmstadt, 德国

DFG Priority Program "Biomimetic Materials Research: Functionality by Hierarchical Structuring of Materials" Winter School

2010年3月23-26日, Kerkrade, 荷兰

International workshop on Coarse-Grained Biomolecular Modeling

2010年3月7-12日, Levi, 芬兰

MolSim 2010 Winter School

2010年1月4-15日, Amsterdam, 荷兰

59th Lindau Nobel Laureate Meeting

2009年6月28日-7月3日, Lindau, 德国

Biomaterials Asia 2009 conference

2009年4月5-8日,香港(会议报告)

学术职务

美国化学会会员

J. Chem. Phys. 等国际权威期刊审稿人