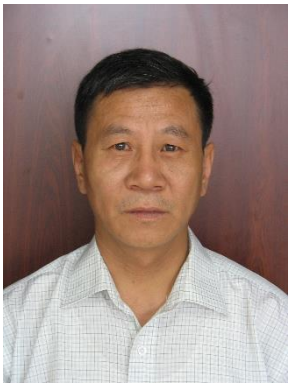
基本信息

姓　　名	**李泽生**	
职　　务		
职　　称	**教授/博士生导师**	
学术兼职	中国化学会理论化学专业委员会委员。《分子科学学报》杂志编委。	
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教育背景

1982.09-1987.07	吉林大学，化学专业，理学硕士/博士
1978.09-1982.07	吉林大学，物理专业，理学学士

工作履历

2010-至今	北京理工大学化学与化工学院，教授
2008-2009	哈尔滨工业大学基础与交叉科学研究院，教授
1987-2007	吉林大学理论化学研究所，讲师/副教授/教授

研究方向

1.	光电转换理论
2.	太阳电池材料的理论设计
3.	光解水催化材料的理论设计

荣誉奖励

1	教育部长江学者特聘教授（2000 年）
2	三次省部级科技进步一等奖

承担项目

1.	染料敏化太阳电池相关材料的设计与计算，科技部 973 课题（2011CBA00701），2011.01-2015.12，400 万元，主持

2.	钙钛矿太阳能电池中电荷输运机理和材料设计的理论研究，国家自然科学基金面上项目（21473010），2015.01-2018.12，85 万元，主持

研究成果

致力于理论化学基础理论及应用。包括量子化学多体理论，高分子固化和标度理论，含时多体理论及应用，重要离子—分子反应微观机理，染料敏化太阳能电池和钙钛矿太阳能电池的理论设计，大气气溶胶表面动力学模拟，生物大分子的结构与功能关系及催化机理的理论研究等领域。主持或作为主要完成人，承担了 20 多项省部级以上科研项目。获得省部级科技进步一等奖三项。发表 SCI 论文 400 多篇。

代表性论文

1.	R. Zhu, Q. S. Li*, Z. S. Li*. Molecular Engineering of Hexaazatriphenylene Derivatives toward More Efficient Electron-Transporting Materials for Inverted Perovskite Solar Cell. ***ACS Appl. Mater. Interfaces.*** 2020, *12*, 38222–38231
2.	B. C. Lu, X. Y. Zheng*, Z. S. Li*. A Promising Photocatalyst of Water Splitting Reaction with Stable Sandwiched P_4O_2/Black Phosphorus Heterostructure and High Solar-to-Hydrogen Efficiency. ***Nanoscale*** 2020, *12*, 6617-6623
3.	J. Yang, Q. S. Li*, Z. S. Li*. End-capped group manipulation of indacenodithienothiophene-based non-fullerene small molecule acceptors for efficient organic solar cells. ***Nanoscale*** 2020, *12*, 17795-17804
4.	M. Y. Hao, W. J. Chi, C. Wang, Z. C. Xu*, Z. S. Li*, X. G. Liu*. Molecular Origins of Photoinduced Backward Intramolecular Charge Transfer. ***J. Phys. Chem. C*** 2020, *124*, 16820–16826
5.	M. Y. Hao, W. J. Chi*, Z. S. Li*. Positional Effect of the Triphenylamine Group on the Optical and Charge-Transfer Properties of Thiophene-Based Hole-Transporting Materials. ***Chem. Asian J.*** 2020, *15*, 287–293
6.	J. Yang, X. L. Peng, Z. Z. Sun, S. Feng, W. L. Ding*, H. Y. He, Z. S. Li*. Understanding the effects of the co-sensitizing ratio on the surface potential, electron injection efficiency, and Forster resonance energy transfer. ***Phys. Chem. Chem. Phys.*** 2020, *12*, 5568-5576
7.	R. Zhu, Q. S. Li*, Z. S. Li*. Introducing pyridyl into electron transport materials plays a key role in improving electron mobility and interface properties for inverted perovskite solar cells. ***J. Mater. Chem. A*** 2019, *7*, 16304–16312
8.	B. C. Lu, X. Y. Zheng* and Z. S. Li*. Few-layer P_4O_2: A Promising Photocatalyst for Water Splitting. ***ACS Appl. Mater. Interfaces.*** 2019, *11*, 10163–10170
9.	R. Zhu, Q. S. Li*, Z. S. Li*. Nitrogen substitution improves the mobility and stability of electron transport materials for inverted perovskite solar cells. ***Nanoscale*** 2018, *10*, 17873-17883
10.	X. X. Ma, Z. S. Li*. The effect of oxygen molecule adsorption on lead iodide perovskite surface by first-principles calculation. ***Appl. Surface Sci.*** 2018, *428*, 140-147

11.	Y. L. Wang, Q. S. Li*, Z. S. Li*. Effect of pi-bridge units on properties of A-pi-D-pi-A-type nonfullerene acceptors for organic solar cells. ***Phys. Chem. Chem. Phys.*** 2018, *20*, 14200-14210
12.	H. J. Zhang, H. Li, L. Liu, Y. Zhang, X. H. Zhang*, Z. S. Li*. The potential role of malonic acid in the atmospheric sulfuric acid - Ammonia clusters formation. ***Chemosphere*** 2018, *203*, 26-33
13.	X. X. Ma, Z. S. Li*. Substituting Cs for MA on the surface of $MAPbI_3$ perovskite: A first-principles study. ***Comput. Mater Sci.*** 2018, *150*, 411-417
14.	W. L. Ding, X. L. Peng, Z. Z. Sun, Z. S. Li*. Novel bifunctional aromatic linker utilized in CdSe quantum dots-sensitized solar cells: boosting the open-circuit voltage and electron injection ***J. Mater. Chem. A*** 2017, *5*, 14319-14330
15.	W. L. Ding, X. L. Peng, Z. Z. Sun, Z. S. Li*. The electron injection rate in CdSe quantum dots sensitized solar cells: From bifunctional linker and zinc oxide morphology ***Nanoscale*** 2017, *9*, 16806-16816
16.	W. J. Chi, D. Y. Zheng, X. F. Chen*, Z. S. Li*. Novel bifunctional aromatic linker utilized in CdSe quantum dots-sensitized solar cells: boosting the open-circuit voltage and electron injection ***J. Mater. Chem. C*** 2017, *5*, 10055-10060
17.	Y. L. Wang, Q. S. Li*, Z. S. Li*. Novel benzodithiophene-based polymer acceptors for efficient organic solar cells. ***Phys. Chem. Chem. Phys.*** 2017, *19*, 23444-23453
18.	P. P. Sun, Q. S. Li*, L. N. Yang, Z. S. Li*. Theoretical insights into a potential lead-free hybrid perovskite: substituting Pb^{2+} with Ge^{2+} ***Nanoscale*** 2016, *8*, 1503-1512
19.	W. J. Chi, Q. S. Li*, Z. S. Li*. Exploring the electrochemical properties of hole transport materials with spiro-cores for efficient perovskite solar cells from first-principles ***Nanoscale*** 2016, *8*, 6146-6154
20.	W. J. Chi, P. P. Sun, Z. S. Li*. A strategy to improve the efficiency of hole transporting materials: introduction of a highly symmetrical core ***Nanoscale*** 2016, *8*, 17752-17756