

基本信息

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职称	教授/博士生导师	
学术兼职	北京化学会副秘书长	
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教育背景

2001.09-2006.06	北京师范大学，物理化学专业，理学博士
1997.09-2001.07	北京师范大学，化学教育专业，理学学士

工作经历

2018.07-至今	北京理工大学化学与化工学院，教授
2013.02-2018.06	北京理工大学化学与化工学院，副教授
2008.05-2012.11	西班牙赫罗纳大学化学系，博士后
2006.07-2008.02	香港城市大学物理与材料科学系，博士后

研究方向

1.	光化学反应机理
2.	光电功能材料的理论设计

荣誉奖励

1	全国高等学校物理化学（含实验）教学微课大赛三等奖（2018年）
2	北京理工大学“优秀青年教师”（2013年）
3	北京理工大学“优秀班主任”（2016年，2017年，2018年）

承担项目

1.	光致变色有机硼化合物反应机理的理论研究，国家自然科学基金面上项目（21773007），2018.01-2021.12，65万元，主持
2.	重氮化合物激发态性质和反应机理的理论研究，国家自然科学基金青年项目（21303007），2014.01-2016.12，25万元，主持

3.	重氮米氏酸沃尔夫重排机理的理论研究，教育部博士点项目 (20131101120053)，2014.01-2016.12，4 万元，主持
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研究成果

运用从头算和动力学模拟方法，研究了多个重要体系的光化学过程，包括聚集诱导发光 (AIE)、沃尔夫重排、含硼光致变色材料的反应机理，等等。探索了多种类型太阳能电池中组件结构和性能的关系，设计了系列高效、稳定、环保的新材料。主持国家自然科学基金项目 2 项和教育部博士点基金一项，参与国家自然科学基金面上项目 1 项。已发表 SCI 论文 70 多篇。

代表性论文

1.	D. Yang, S. K. Mellerup, J. B. Peng, X. Wang, Q. S. Li* , S. Wang*. Substituent directed phototransformations of BN-heterocycles: elimination vs isomerization via selective B-C bond cleavage. <i>J. Am. Chem. Soc.</i> 2016, <i>138</i> , 11513-11516
2.	S. K. Mellerup, C. Li, J. Radtke, X. Wang, N. Wang*, Q. S. Li* , S. Wang*. Photochemical generation of chiral N,B,X - heterocycles by heteroaromatic C-X bond scission (X=S, O) and boron insertion. <i>Angew. Chem. Int. Ed.</i> 2018, <i>57</i> , 9634-9639
3.	S. Wang*, K. Yuan, M. F. Hu, X. Wang, T. Peng, N. Wang*, Q. S. Li* . Cleavage of unstrained C-C bonds in acenes by boron and light: transformation of naphthalene into benzoborepin. <i>Angew. Chem. Int. Ed.</i> 2018, <i>57</i> , 1073-1077
4.	R. Zhu, Q. S. Li* , Z. S. Li*. Molecular engineering of hexaazatriphenylene derivatives toward more efficient electron-transporting materials for inverted perovskite solar cell. <i>ACS Appl. Mater. Interfaces.</i> 2020, <i>12</i> , 38222-38231
5.	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. <i>Nanoscale</i> 2020, <i>12</i> , 17795-17804
6.	X. Y. Du, Q. S. Li* . Theoretical study on photoisomerization mechanisms of diphenyl-substituted N,C-chelate organoboron compounds. <i>Chem. Eur. J.</i> 2020, <i>26</i> , 12891-12897
7.	H. Y. Zhu, Q. S. Li* . Insights into the photoinduced isomerization mechanisms of a N,C-chelate organoboron compound: a theoretical study. <i>ChemPhysChem</i> 2020, <i>21</i> , 510-517
8.	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. <i>J. Mater. Chem. A</i> 2019, <i>7</i> , 16304-16312
9.	F. P. Li, H. Y. Zhu, Q. S. Li* , Z. S. Li*. Theoretical study on the regioselective photoisomerization of asymmetric N,C-chelate organoboron compounds. <i>Phys. Chem. Chem. Phys.</i> 2019, <i>21</i> , 8376-8383
10.	W. L. Ding, X. L. Peng, G. L. Cui, Z. S. Li*, L. Blancafort*, Q. S. Li* . Potential-energy surface and dynamics simulation of THBDBA: an annulated tetraphenylethene derivative combining aggregation-induced emission and switch

	behavior. <i>ChemPhotoChem</i> 2019, 3, 814-824
11.	R. Zhu, Q. S. Li* , Z. S. Li*. Nitrogen substitution improves the mobility and stability of electron transport materials for inverted perovskite solar cells. <i>Nanoscale</i> 2018, 10, 17873-17883
12.	J. Bai, B. Lu, Q. Han*, Q. S. Li* , L. Qu*. (111) Facets-oriented Au-decorated carbon nitride nanoplatelets for visible-light-driven overall water splitting. <i>ACS Appl. Mater. Interfaces</i> . 2018, 10, 38066–38072
13.	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. <i>Phys. Chem. Chem. Phys.</i> 2018, 20, 14200-14210
14.	X. L. Peng, A. Migani, Q. S. Li* , Z. S. Li, L. Blancafort*. Theoretical study of non-Hammett vs. Hammett behaviour in the thermolysis and photolysis of arylchlorodiazirines. <i>Phys. Chem. Chem. Phys.</i> 2018, 20, 1181-1188
15.	X. L. Peng, W. L. Ding, Q. S. Li* , Z. S. Li*. Theoretical insights into photo-induced Curtius rearrangement of chlorodifluoroacetyl azide. <i>Org. Chem. Front.</i> 2017, 4, 1153-1161
16.	W. J. Wu, Q. S. Li* , Z. S. Li *. Insights into the thermal eliminations and photoeliminations of B,N-heterocycles: a theoretical study. <i>J. Phys. Chem. A</i> 2017, 4, 753-761
17.	Y. L. Wang, Q. S. Li* , Z. S. Li*. Novel benzodithiophene-based polymer acceptors for efficient organic solar cells. <i>Phys. Chem. Chem. Phys.</i> 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⁺ <i>Nanoscale</i> 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 <i>Nanoscale</i> 2016, 8, 6146-6154
20.	X. L. Peng, S. Ruiz-Barragan, Z. S. Li, Q. S. Li* , L. Blancafort*. Restricted access to a conical intersection to explain aggregation induced emission in dimethyl tetraphenylsilole. <i>J. Mater. Chem. C</i> 2016, 4, 2802–2810