CURRICULUM VITAE

WENQING ZHANG（张文清）

Department of Materials Science and Engineering,

1088 Xueyuan Rd., Shenzhen, Guangdong, 518055, China

Phone: 86-0755-88018220,13764943712

Email: [zhangwq@sustech.edu.cn](mailto:zhangwq@sustech.edu.cn)

Research ID: <http://www.researcherid.com/rid/K-1236-2012>

# TITLE Full Professor in Materials Science and Engineering, SUSTech

# EDUCATION

1992 Ph. D., Physics, Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, China: “Interaction of atoms with strong converging laser field” (advisor: Professor Weihan Tan)

1989 M. S., physics, Xiamen University, China

1986 B. S., physics, Xiamen University, China

#### POSITIONS

2021 - Present Professor, Department of Materials Science and Engineering

Southern University of Science and Technology

2017 - 2021 Professor, Department of Physics

Southern University of Science and Technology

2014 - 2017 Professor, Material Genome Institute, Shanghai University

2011 - 2014 Professor, Group Leader, School of Chemistry and Chemical

Engineering, Nanjing University, Jiangsu, China

2003 - 2011 Professor, Group Leader, Deputy Director of the State Key Laboratory of High Performance Ceramics and Superfine Microstructures, Shanghai Institute of Ceramics, Chinese Academy of Sciences, Shanghai 200050, China

2004 - 2005 Visiting Professor, Institute for Metal Research, Max-Planck-Gesellschaft, Stuttgart, Germany

1997 - 2003 Research staff, Physics and Physical Chemistry Department, General Motors R&D, Warren, Michigan, USA

2002 - 2003 Research Faculty, Materials Department, University of California, Santa Barbara, Santa Barbara, CA 93106

2000 - 2002 Research Staff, Princeton Materials Institute, Princeton University, Princeton, NJ 0854

1997 - 1999 Research Associate Fellowship, Division of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138

1997 Visiting Scientist, Theory Department, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin-Dahlem, Germany

1995-1997 Associate Professor, Institute of Applied Physics, Beijing University of Science & Technology, China

1993-1995 Postdoctoral Researcher, Institute of Physics, Chinese Academy of Science, China (Supervisor: Professor Dingsheng Wang)

# AWARDS AND HONORS

2020 Zhujiang Scholarship，珠江人才-领军人才项目

2018 Zhujiang Scholar Research Team Project (Guangdong Province)

珠江人才项目，广创团队负责人

2017 Pengcheng Scholar (Shenzhen city) 深圳鹏城学者

2015 Shanghai Excellent Science Discipline Leader 上海市学科带头人

2014 Fellow, American Physical Society， 美国物理学会会士

2013 The State Natural Science Award, China, Second rank

国家自然科学二等奖（排名第二）

2012 Shanghai Municipal Natural Science Award, First-rank

上海自然科学一等奖（排名第二）

2010 Outstanding Scientists and Engineers of China 国家百千万人才

2008 Exceptional Young Scientist Foundation Award from NSFC

自然科学基金委杰出青年基金项目

2004 “One-hundred-Talent Plan” from Chinese Academy of Sciences

中科院百人计划项目

##### PROFESSIONAL MEMBERSHIP, ACTIVITY, AND SERVICE

**Membership**

1997-present Member, American Physical Society

1997-present Member, American Materials Research Society

**Symposium Organizer**

2021 Symposium Organizer，Symposium on Functional Units and Construction rules（基元序构） for Advanced Functional Materials Design, Shenzhen, China

2017-2020 Co-organizers (with Prof. Zhong FANG, Prof. Xin-gao GONG, amd Prof. Xi DAI), Annual Workshop on Computational Physics (Shenzhen, 2017; Xiamen, 2018; Shandou, 2019).

2016 Symposium Organizer (with Prof. Jiangyu Li), Symposium on Mechanical integrity of Energy conversion and storage materials, Phoenix, USA

2013 Symposium Organizer, Symposium on Thermoelectrics, Materials Research Society Fall Meeting, Boston, USA

2010 Co-Organizer, 27th International Conference on Thermoelectrics, 2010, Shanghai, China

2010 Organizer, Workshop on “Thermoelectric Transport Fundamentals”, the 2nd Shanghai International Workshop on High-performance Ceramics, Hangzhou, China

2008 Symposium Organizer, Symposium on “Engineering Interfaces for New Materials: Modeling and Experiments”, Annual Meeting of the Physical Society of America (APS’2008), New Orleans, USA

2007 Symposium Organizer, Symposium on “Thermoelectric Materials and Devices”, the 7th Pacific-rim Conference on Advanced Ceramics, Shanghai, China,

2007 Organizer, Forum on “Advanced Thermoelectric Materials and Devices”, the 1st Shanghai International Forum on Advanced Materials, Shanghai, China

2006 Co-chair: Symposium on “Fundamental Research on Energy-conversion Materials”, the 5th annual meeting of the Overseas Chinese Physics Association (OCPA5), Taipei, China

**Services**

2022-present Editorial Board Member, NSO -Natural Science Open

2017-present Associate Editor, Applied Physics Letters

2015-present Editorial Board Member, npj Computational Materials

2014-present Editorial Board Member, Journal of Materiomics

2014-2016 Guest Editor, Journal of Electronic Materials

2014-Present Vice-Chairman, Sub-committee of Thermoelectric Materials, CMRS

2010-Present Vire-Chairman, Sub-committee of Computational Materials Science and Computational Physics, CMRS

2014-2017 Deputy Director of Material Genome Institute, Shanghai University

2010-2013 Deputy Director of the State Key Laboratory of High Performance Ceramics and Superfine Microstructures, Shanghai Institute of Ceramics

2007-present Member, Scientific Advisory Committee, Shanghai Institute of Ceramics

2010-present Member, Scientific Advisor Committee, MOE-key Laboratory of Computational Physics and Computational Mathematics, Fudan University

2010-present Member, Scientific Advisor Committee, MOE-key Laboratory of Quantum Phenomenon and Condensed Matter Physics, Shanghai Jiaotong University

2010-present Board Member, International Thermoelectric Society

2010-2011 Guest Editor, Journal of Electronic Materials

2008-present Member, Editorial Board, Chinese Physics Letter

2010-present Board Member, Thermoelectric Materials and Device Division, Chinese Materials Research Society

2010-present Board Member, Computational Physics Division, Chinese Nuclear Physics Society

2005-present Board Member, Computational Materials Science and Physics Division, Chinese Materials Research Society

2005-2006 Proceedings and Books Subcommittee, Materials Research Society

**Reviewer for**

Physical Review Letters, Nature Communication, PNAS, Advanced Materials, Advanced Functional Materials, Energy & Environmental Sci., Physical Review B, Applied Physics Letters, Journal of Applied Physics, Journal of Alloys and Compounds, Journal of Electronic Materials, Journal of Solid State Chemistry, Chinese Physics Letters, Journal of Physics: Cond Matter, Physics B, Journal of America Chemistry Society, Chemistry of Materials, Nanoscale, Chem. Mater.

**Grand Proposal Reviewer for**

National Nature Science Foundation of China

National Basic Research Program of China (973)

National Science Foundation, USA

##### PUBLICATION LIST

##### Invited Reviews and Book Chapters

1. 张莉\*, 王继扬, 张文清, 陈延峰, 张清杰. 材料交叉前沿战略研究. 武汉理工大

学出版社，2021.

1. Jiong Yang, Yancheng Wang, Hongliang Yang, Wei Tang, Jihui Yang, Lidong Chen, **Wenqing Zhang\***, Thermal transport in thermoelectric materials with chemical bond hierarchy, Journal of Physics-Condensed Matter, 2019, 31(18), 183002.

15. Fang, Xin Li, Chaoliang Hu, Qi Zhang, Jiong Yang\*, **Wenqing Zhang**, Xinbing Zhao\*, David J. Singh, Tiejun Zhu\*, Complex Band Structures and Lattice Dynamics of Bi2Te3‐Based Compounds and Solid Solutions, Advanced Functional Materials, 2019, 29, 1900677.

14. Lu, Wencong, Ruijuan Xiao, Jiong Yang, Hong Li, and **Wenqing Zhang**. "Data mining-aided materials discovery and optimization." Journal of Materiomics 2017, 3, 191-201.

13. Youwei Wang, Wujie Qiu, Erhong Song, Feng Gu, Zhihui Zheng, Xiaolin Zhao, Yingqin Zhao, Jianjun Liu, **Wenqing Zhang**; Adsorption-energy-based activity descriptors for electrocatalysts in energy storage applications, National Science Review, 5, 327–341 (2018).

12. J. Yang, L. Xi, W. Qiu, L. Wu, X. Shi, L. Chen, J. Yang, **W. Zhang**, C. Uher, D. J. Singh, On the tuning of electrical and thermal transport in thermoelectrics: an integrated theory-experiment perspective, NPJ Computational Materials, 2, 15015 (2016).

11. L. Xi, J. Yang, L. Wu, J. Yang, **W. Zhang**. Band Engineering and Rational Design of High Performance Thermoelectric Materials from First-Principles, Journal of Materiomics 2, 114(2016).

10. W. Qiu, X. Ke, L. Xi, L. Wu, J. Yang, **W. Zhang**, Sci. China Phys. Mech. Astron. 59, 627001 (2016).

9. 孙永兴, 杨炯, 席丽丽, 邱吴劼, 吴立华, **张文清**. 电热输运微观机制理解与新热电材料设计.自然杂志, 38(5), 327-333 (2016).

8. 吴立华, 杨炯, 李鑫, 骆军, **张文清**. 热电材料中自旋轨道耦合效应对电输运的影响.自然杂志, 38(5), 320-326 (2016).

7. 席丽丽, 邱雨婷, 史迅, 杨炯, 陈立东, 杨继辉, **张文清**. CoSb3基方钴矿化合物的 Ga, In 掺杂及相关复杂缺陷的研究.中国材料进展, 34(1), 41-49 (2015).

6. J. Yang, L. Xi, **W. Zhang**, L.D. Chen, D. Wang, and Z.G. Shuai, “Band Engineering and Design of Thermoelectric Materials”, *Modeling and Simulation of Materials at Nanoscale*, Eds. Z. Shuai, and K. Xia, (Beijing, Scientific publisher, 2013) ;杨炯，席丽丽，**张文清**，陈立东，王冬，帅志刚，“基于理论计算的能带调控及热电材料设计”，纳米结构与性能的理论计算及模拟，帅志刚，夏钶等著，北京，科学出版社，2013.

5. L.D. Chen, Z. Xiong, R.H. Liu, **W. Zhang**, “Bulk Nanocomposites of Thermoelectric Materials”, *Materials, Preparation, and Characterization in Thermoelectrics*, Edited by D. M. Rowe, CRC Press, 2012.

4. J. Yang, X. Shi, **W. Zhang**, L.D. Chen, J. Yang, “Ab Initio-Based Band Engineering and Rational Design of Thermoelectric Materials”, *Materials, Preparation, and Characterization in Thermoelectrics*, Edited by D. M. Rowe, CRC Press, 2012.

3. X. Shi, S.Q. Bai, L. Xi, J. Yang, **W. Zhang**, L,D. Chen, J. Yang, “Realization of high thermoelectric performance in n-type partially filled skutterudites”, J. Mater. Res. 26, 1745-1755 (2011).

2. L.L.Xi, J. Yang, X. Shi, **W. Zhang**, L.D. Chen and J.H. Yang, “Filled skutterudites:from single to multiple filling”, Scientia Sinica Physica, 41 (2011), 706-728. (席丽丽，杨炯，史迅，**张文清**，陈立东，杨继辉，“填充方钴矿热电材料：从单填到多填”，中国科学，41(6), 706-728 (2011).

1. L. Xi, **W. Zhang**, L. Chen, and J. Yang, “Filled Skutterudites: from single to multiple filling”, J. Kor. Ceram. Soc., 47, 54-60 (2010).

##### Refereed Journal （Until Sept. 2022）

（Full list & citation, see Research ID: <http://www.researcherid.com/rid/K-1236-2012>）

More than 280 papers published, including more than 100 papers published after joining SUStech in July, 2017

284. Zirui Dong, Jun Luo\*, Chenyang Wang, Ying Jiang, Shihua Tan, Yubo Zhang, Yuri Grin, Zhiyang Yu, Kai Guo, Jiye Zhang **Wenqing Zhang**\*, ‘Half-Heusler-like compounds with wide continuous compositions and tunable p- to n-type semiconducting thermoelectrics’ Nature Communications, 2022, 12-15

283. Xingwei Zheng, Jian Cui, Chao Gu, Weichao Bao, Xuefeng Zhou, Ji-XuanLiu\*, Guo-Jun Zhang, Wenqing Zhang, Yusheng Zhao, Shanmin Wang\*, Yongcheng Liang, ‘Superhard high-entropy dodecaboride with high electrical conductivity’, 2022, 220, 114938

282. Erting Dong, Yongbin Zhu, Shihua Tan, Weishu Liu, Jiong Wang, **Wenqing Zhang**\*, ‘Bistructural Pseudocontinuous Solid Solution with Hierarchical Microstructures from Ab initio Study: Application to the Mg2Sn−Mg3Sb2 System’, Acta Materialia, 2022, 236, 118139

281. Yabei Wu, Zhao Tang, Greis J. Cruz, Ya Yang, **Wenqing Zhang**, Wei Ren\*, and Peihong Zhang\*, ‘Exploiting the stereoelectronic effects for selective tuning of band edge states of α-SnO: GW quasiparticle calculations’ Phys. Rev. B, 2022, 106, 085201

280. Pin Chen, Jianwen Chen, Hui Yan, Qing Mo, Zexin Xu, Jinyu Liu, Wenqing Zhang, Yuedong Yang\*, Yutong Lu\*, ‘Improving Material Property Prediction by Leveraging the Large-Scale Computational Database and Deep Learning’ The Journal of Physical Chemistry C, 2022

279. Yifan Liu, Caichao Ye, Shu-Na Zhao, Yunyan Wu, Chao Liu, Jiangfeng Huang, Liang Xue, Jingwen Sun, Wenqing Zhang, Xin Wang, Pan Xiong\*, Junwu Zhu\*, ‘A dual-site doping strategy for developing efficient perovskite oxide electrocatalysts towards oxygen evolution reaction’, Nano Energy, 2022, 99, 107344

278. Rui Shu, Zhijia Han, Anna Elsukova, Yongbin Zhu, Peng Qin, Feng Jiang, Jun Lu, Per O Å Persson, Justinas Palisaitis, Arnaud le Febvrier, **Wenqing Zhang**, Oana Cojocaru-Mirédin, Yuan Yu , Per Eklund, Weishu Liu, ‘Solid‐State Janus Nanoprecipitation Enables Amorphous‐Like Heat Conduction in Crystalline Mg3Sb2‐Based Thermoelectric Materials’ Advanced Science, 2022, 9(5)

277. Zhou Zhang, Yifan Zhu, Jialin Ji, Jianxin Zhang, Huifang Luo, Chenguang Fu, Qianqian Li, Madison Brod, G. Jeffrey Snyder, Yubo Zhang, Jiong Yang\*, **Wenqing Zhang**, ‘Ag rearrangement induced metal-insulator phase transition in thermoelectric MgAgSb’ Materials Today Physics, 2022, 25, 100702

276. Luyao Wang, Zirui Dong, Shihua Tan, Jiye Zhang, Wenqing Zhang, Jun Luo\*, ‘Discovery of a Slater–Pauling Semiconductor ZrRu1.5Sb with Promising Thermoelectric Properties’ Advanced Functional Materials, 2022, 32(25)

275. Cong Su, Fang Zhang, Salman Kahn, Brian Shevitski, Jingwei Jiang, Chunhui Dai, Alex Ungar, Ji-Hoon Park, Kenji Watanabe, Takashi Taniguchi, Jing Kong, Zikang Tang, **Wenqing Zhang**, Feng Wang, Michael Crommie, Steven G. Louie\*, Shaul Aloni\*, Alex Zettl\*, ‘Tuning colour centres at a twisted hexagonal boron nitride interface’ Nat Mater., 2022, 21(8):896-902

274. Yabei Wu, Zhao Tang, Weiyi Xia, Weiwei Gao, Fanhao Jia, Yubo Zhang, Wenguang Zhu, **Wenqing Zhang\***, Peihong Zhang\*, ‘Prediction of protected band edge states and dielectric tunable quasiparticle and excitonic properties of monolayer MoSi2N4’ npj Computational Materials, 2022, 129

273. Yan Cao, Zhenyu Zhu, Xin Li, Jinyang Xi, David J. Singh, Lili Xi\*, Jiong Yang\*, **Wenqing Zhang,** ‘Unraveling the relationships between chemical bonding and thermoelectric properties: n-type ABO(3) perovskites’ J. Mater. Chem. A, 2022,10, 11039-11045

272. Zhao Tang, Greis J. Cruz, Yabei Wu, Weiyi Xia, Fanhao Jia, **Wenqing Zhang**, Peihong Zhang\*, ‘Giant Narrow-Band Optical Absorption and Distinctive Excitonic Structures of Monolayer C3N and C3B’, PHYS. REV. APPLIED, 202217, 034068

271.Yunyan Wua, Caichao Ye, Lei Yua, Yifan Liua, Jiangfeng Huang, Jiabao Bi, Liang Xue, Jingwen, Sun, Juan Yang, **Wenqing Zhang**, Xin Wang, Pan Xiong, Junwu Zhu\*, ‘Soft template-directed interlayer confinement synthesis of a Fe-Co dual single-atom catalyst for Zn-air batteries’ Energy Storage Materials, 2022, 45, 805-813

270. Luyao Wang, Zirui Dong, Shihua Tan, Jiye Zhang, Wenqing Zhang, and Jun Luo\*, ‘Discovery of a Slater–Pauling Semiconductor ZrRu1.5Sb with Promising Thermoelectric Properties’ Adv. Funct. Mater. 2022, 2200438

269. Jizhang Chen\*, Minfeng Chen, Weijun Zhou, Xinwu Xu, Bo Liu\*, Wenqing Zhang, and Chingping Wong\*, ‘Simplified Synthesis of Fluoride-Free Ti3C2Tx via Electrochemical Etching toward HighPerformance Electrochemical Capacitors’ ACS Nano 2022, 16, 2461−2470

268. Xiang Han, Weijun Zhou, Minfeng Chen, Linshan Luo, Lanhui Gu, Qiaobao Zhang, Jizhang Chen\*, Bo Liu\*, Songyan Chen\*, **Wenqing Zhang** ‘Liquid-phase sintering enabling mixed ionic-electronic interphasesand free-standing composite cathode architecture toward high energy solid-state battery’, Nano Research 2022, 15, 6156–6167

267. Tao Feng, Panshuo Wang, Zhijia Han, Liang Zhou, **Wenqing Zhang\*,** Qihang Liu\*, and Weishu Liu\*, ‘Large Transverse and Longitudinal Magneto-Thermoelectric Effect in Polycrystalline Nodal-Line Semimetal Mg3Bi2’, Advanced Materials, 2022, 2200931

265. Hao Chen, Minfeng Chen, Weijun Zhou, Xiang Han, Bo Liu, **Wenqing Zhang,** Jizhang Chen\*, ‘Flexible Ti3C2Tx/Nanocellulose Hybrid Film as a Stable Zn-free Anode for Aqueous Hybrid Zn−Li Batteries’ ACS Appl. Mater. Interfaces 2022, 14, 6876−6884

264.Jinyang Xi, Liangliang Zheng, Shenghao Wang, Jiong Yang\*, and **Wenqing Zhang**\*, ‘Temperature-Dependent Structural Fluctuation and Its Effect on the Electronic Structure and Charge Transport in Hybrid Perovskite CH3NH3PbI3’, Journal of Computational Chemistry, 2021, 42, 2213–2220

263.Wenting Wu, Huajing Fang\*, Hailong Ma, Liangliang Wu, **Wenqing Zhang**, and Hong Wang\*, ‘Correction to: Boosting Transport Kinetics of Ions and Electrons Simultaneously by Ti3C2Tx (MXene) Addition for Enhanced Electrochromic Performance’, Nano-Micro Letters, 2021, 13, 214

262.Lei Hu, Yubo Luo, Yue-Wen Fang, Feiyu Qin, Xun Cao, Hongyao Xie, Jiawei Liu, Jinfeng Dong, Andrea Sanson, Marco Giarola, Xianyi Tan, Yun Zheng, Ady Suwardi, Yizhong Huang, Kedar Hippalgaonkar, Jiaqing He, **Wenqing Zhang**, Jianwei Xu, Qingyu Yan\*, and Mercouri G. Kanatzidis\*, ‘High Thermoelectric Performance through Crystal Symmetry Enhancement in Triply Doped Diamondoid Compound Cu2SnSe3’, Advanced Energy Materials, 2021, 11, 2100661

261.Xiaozhe Zhang, Na Li, Jun Zhang, Yanshen Zhang, Xiaoli Yang, Yifan Luo, Bobo Zhang, Zhixue Xu, Zhenhua Zhu, Xiuyan Yang, Yuan Yan, Biao Lin, Shen Wang, Da Chen, Caichao Ye, Yan Ding, Mingliang Lou, Qingcui Wu, Zhanfeng Hou, Keren Zhang, Ziming Liang, Anqi Wei, Bianbian Wang, Changhe Wang, Nan Jiang, **Wenqing Zhang**, Guozhi Xiao, Cong Ma, Yan Ren, Xiangbing Qi, Weiping Han, Chao Wang\*, and Feng Rao\*, ‘5-IP7 Is a GPCR Messenger Mediating Neural Control of Synaptotagmin-Dependent Insulin Exocytosis and Glucose Homeostasis’, Nature Metabolism, 2021, 3, 1400–1414

260.Hongliang Yang, Yifan Zhu, Erting Dong, Yabei Wu, Jiong Yang\*, and **Wenqing Zhang**\*, ‘Dual Adaptive Sampling and Machine Learning Interatomic Potentials for Modeling Materials with Chemical Bond Hierarchy’, Physical Review B, 2021, 104, 094310

259.Yongbin Zhu, Erting Dong, Zhijia Han, Feng Jiang, Jiehe Sui, **Wenqing Zhang**\*, and Weishu Liu\*, ‘Maximized Atomic Disordering Approach Boost the Thermoelectric Performance of Mg2Sn through the Self-Compensation Effect and Steric Effect’, Acta Materialia, 2021, 217, 117172

258.Bo Liu\*, Tianyu Gao, Peiguang Liao, Yufeng Wen, Mingjia Yao, Siqi Shi\*, and **Wenqing Zhang**, ‘Metallic VS2/Graphene Heterostructure as an Ultra-High Rate and High-Specific Capacity Anode Material for Li/Na-Ion Batteries’, Physical Chemistry Chemical Physics, 2021, 23 (2021), 18784–18793

257.Mingjia Yao, Yuxiang Wang, Xin Li, Ye Sheng, Haiyang Huo, Lili Xi, Jiong Yang \*, and **Wenqing Zhang**, ‘Materials Informatics Platform with Three Dimensional Structures, Workflow and Thermoelectric Applications’, Scientific Data, 2021, 8, 236

256.Xiang Han, Shanyu Wang, Yaobin Xu, Guiming Zhong, Yang Zhou, Bo Liu, Xiaoyu Jiang, Xiang Wang, Yun Li, Ziqi Zhang, Songyan Chen, Chongmin Wang, Yong Yang, **Wenqing Zhang**, Junlan Wang, Jun Liu\* and Jihui Yang\*, ‘All Solid Thick Oxide Cathodes Based on Low Temperature Sintering for High Energy Solid Batteries’, Energy & Environmental Science, 2021, 14, 5044–5056

255.Erting Dong, Shihua Tan, Jiong Wang, Weishu Liu, and **Wenqing Zhang**\*, ‘Thermodynamic Activity of Solute in Multicomponent Alloy from First-Principles: Excess Mg in Mg3(Sb1-xBix)2 as an Example’, Calphad, 2021, 74, 102318

254.Chao Gu, Yongcheng Liang\*, Xuefeng Zhou, Jian Chen, Dejiang Ma, Jiaqian Qin, **Wenqing Zhang**, Qiang Zhang, Luke L. Daemen, Yusheng Zhao, and Shanmin Wang, ‘Crystal Structures and Formation Mechanisms of Boron-Rich Tungsten Borides’, Physical Review B, 2021, 104, 014110

253.Hui Luo, Songhao Guo, Yubo Zhang, Kejun Bu, Haoran Lin, Yingqi Wang, Yanfeng Yin, Dongzhou Zhang, Shengye Jin, **Wenqing Zhang**, Wenge Yang, Biwu Ma, and Xujie Lü\*, ‘Regulating Exciton–Phonon Coupling to Achieve a Near-Unity Photoluminescence Quantum Yield in One-Dimensional Hybrid Metal Halides’, Advanced Science, 2021, 8 (2021), 2100786

252.Shiyang He, Yang Yang, Zhili Li, Jiye Zhang, Chenyang Wang, **Wenqing Zhang**, and Jun Luo\*, ‘A General Strategy for High-Throughput Experimental Screening of Promising Bulk Thermoelectric Materials’, Science China Materials, 2021, 64, 1751–1760

251.Yuanqing Mao, Hongliang Yang, Ye Sheng, Jiping Wang, Runhai Ouyang, Caichao Ye\*, Jiong Yang\*, and **Wenqing Zhang**, ‘Prediction and Classification of Formation Energies of Binary Compounds by Machine Learning: An Approach without Crystal Structure Information’, ACS Omega, 2021, 6, 14533–14541

250.Haiyang Huo, Yuxiang Wang, Lili Xi\*, Jiong Yang\*, and **Wenqing Zhang**, ‘The Variation of Intrinsic Defects in XTe (X = Ge, Sn, and Pb) Induced by the Energy Positions of Valence Band Maxima’, Journal of Materials Chemistry C, 2021, 9, 5765–5770

249.Yongcheng Liang, Xiao-Feng Wei, Chao Gu, Ji-Xuan Liu, Fei Li, Mingqi Yan, Xingwei Zheng, Zhilin Han, Yusheng Zhao, Shanmin Wang\*, Jiong Yang, **Wenqing Zhang**, Liangzhi Kou, and Guo-Jun Zhang\*, ‘Enhanced Hardness in Transition-Metal Monocarbides via Optimal Occupancy of Bonding Orbitals’, ACS Applied Materials & Interfaces, 2021, 13 (2021), 14365–14376

248.Can Yang, Chongze Hu, Congying Xiang, Hongbo Nie, Xinfu Gu, Lin Xie, Jiaqing He, **Wenqing Zhang**, Zhiyan Yu\*, and Jian Luo\*, ‘Interfacial Superstructures and Chemical Bonding Transitions at Metal-Ceramic Interfaces’, Science Advances, 2021

247.Pan, S., L. Liu, Z. Li, X. Yan, C. Wang, K. Guo, J. Yang\*, J. Luo\*, and **W. Zhang**, ‘Embedded In-Situ Nanodomains from Chemical Composition Fluctuation in Thermoelectric A2Cu3In3Te8 (A= Zn, Cd)’, Materials Today Physics, 2021, 17, 100333

246.Ziyu Wang, Jinyang Xi, Jinyan Ning, Kai Guo, Bo Duan, Jun Luo, G. Jeffrey Snyder, Jiong Yang\*, and **Wenqing Zhang**\*, ‘Temperature-Dependent Band Renormalization in CoSb3 Skutterudites Due to Sb-Ring-Related Vibrations’, Chemistry of Materials, 2021, 33, 1046–1052

245.Bing He, Penghui Mi, Anjiang Ye, Shuting Chi, Yao Jiao, Liwen Zhang, Bowei Pu, Zheyi Zou, **Wenqing Zhang**, Maxim Avdeev, Stefan Adams, Jingtai Zhao, and Siqi Shi\*, ‘A Highly Efficient and Informative Method to Identify Ion Transport Networks in Fast Ion Conductors’, Acta Materialia, 2021, 203, 116490

244.Shihua Tan, Pengfei Nan, Kaiyang Xia, Hongliang Yang, Tiejun Zhu, Binghui Ge\*, and **Wenqing Zhang**\*, ‘Sublattice Short-Range Order and Modified Electronic Structure in Defective Half-Heusler Nb0.8CoSb’, The Journal of Physical Chemistry C, 2021, 125 (2021), 1125–1133

243.Mao Ye, Songbai Hu, Yuanmin Zhu, Yubo Zhang, Shanming Ke\*, Lin Xie, Yuan Zhang, Sixia Hu, Dongwen Zhang, Zhenlin Luo, Meng Gu, Jiaqing He, Peihong Zhang, **Wenqing Zhang**, and Lang Chen\*, ‘Electric Polarization Switching on an Atomically Thin Metallic Oxide’, Nano Letters, 2021, 21, 144–150

242.Xin Li, Zhou Zhang, Jinyang Xi, David J. Singh, Ye Sheng, Jiong Yang\*, and **Wenqing Zhang**, ‘TransOpt. A Code to Solve Electrical Transport Properties of Semiconductors in Constant Electron–Phonon Coupling Approximation’, Computational Materials Science, 2021, 186 (2021), 110074

241.Yongbin Zhu, Zhijia Han, Feng Jiang, Erting Dong, Bo-Ping Zhang, **Wenqing Zhang**\*, and Weishu Liu\*, ‘Thermodynamic Criterions of the Thermoelectric Performance Enhancement in Mg2Sn through the Self-Compensation Vacancy’, Materials Today Physics, 2021, 16, 100327

240.Xin Li, Ye Sheng, Lihua Wu, Shunbo Hu, Jiong Yang\*, David J. Singh, Jihui Yang, and **Wenqing Zhang\*,** “Defect-mediated Rashba engineering for optimizing electrical transport in thermoelectric BiTeI”, NPJ Computational Materials, 2020, 6, 107,

239.Zichen Wei, Chenyang Wang\*, Jiye Zhang, Jiong Yang, Zhili Li, Qidong Zhang, Pengfei Luo, **Wenqing Zhang**, Enke Liu\*, and Jun Luo\*, “Precise regulation of carrier concentration in thermoelectric BiSbTe alloys via magnetic doping”, ACS Appl. Mater. Interfaces, 2020, 12, 20653-20663,

238.Bo Liu, Da Wang, Maxim Avdeev, Siqi Shi\*, Jiong Yang\*, and **Wenqing Zhang\***, “High-Throughput Computational Screening of Li-Containing Fluorides for Battery Cathode Coatings”, ACS Sustainable Chemistry & Engineering, 2020,8, 948-957

237.Bo Liu, Jian Liu, Jiong Yang, Da Wang, Caichao Ye, Deyu Wang, Maxim Avdeev, Siqi Shi\*, Jihui Yang\*, and **Wenqing Zhang\*,** “Ab initio thermodynamic optimization of Ni-rich Ni-Co-Mn oxide cathode coatings”, Journal of Power Sources, 2020, 450, 227693,

236.Youwei Wang, Junkai Wang, Xiaolin Zhao, Wujie Qiu, Erhong Song, **Wenqing Zhang**, Xiangfeng Liu and Jianjun Liu, Reducing the charge overpotential of Li–O2 batteries through band-alignment cathode design. Energy & Environmental Science， 2020,

235.Lili Zhang, Gang Wang, Yubo Zhang, Zhipeng Cao, Yu Wang, Tianjun Cao, Cong Wang, Bin Cheng, **Wenqing Zhang**, Xiangang Wan, Junhao Lin\*, Shi-Jun Liang\*, and Feng Miao\*, Tuning Electrical Conductance in Bilayer MoS2 through Defect-Mediated Interlayer Chemical Bonding, American Chemical Society,2020,

234.Zhishan Luo, Chongze Hu, Lin Xie, Hongbo Nie, Congying Xiang, Xinfu Gu, Jiaqing He, **Wenqing Zhang\***，Zhiyang Yu\*，and Jian Luo\*，A highly asymmetric interfacial superstructure in WC: expanding the classic grain boundary segregation and new complexion theories†, Materials Horizons, 2020, 7, 173—180.

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6. 罗宏杰; 骆军; 张继业; 曹世勋; 吴立华; 张文清; 二维连续成分样品、其制备方法及其在相图高通快速测定中的应用, 2018.10.23, 中国, ZL201610188226.8. （授权发明专利）

5. 罗宏杰; 骆军; 吴立华; 张继业; 曹世勋; 张文清; 基于连续成分块材的高通量热电性能表征方法及其应用, 2018.08.17, 中国, ZL201610188029.6. （授权发明专利）

4. 陈立东; 仇鹏飞; 刘睿恒; 张文清; 黄向阳; 史迅; 杨炯; 何琳; 空穴补偿型方钴矿热电材料及其制备方法, 2015.11.25, 中国, ZL201110194902.X （授权发明专利）

3. L.D. Chen, R.H. Liu, P.F. Qiu, **W. Zhang**, X.Y. Huang, J. Yang, L. He et al., High-Efficiency p-type Skuterudites, China patent, 201010259433.0, 陈立东、刘睿恒、仇鹏飞、张文清、黄向阳、杨炯、何琳、莫尼卡·拜克浩斯，p型方钴矿材料及其制备方法，中国发明专利(Chinese Patent Application)，201010259433.0

2. L.D. Chen, Z. Xiong, X.H. Chen, X.Y. Huang, **W. Zhang**, L. He, 陈立东、熊震、陈喜红、黄向阳、张文清、何琳，一种填充方钴矿基复合材料及其制备方法，中国发明专利(Chinese Patent Application)，200910196619.3.

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**Published Applications**

3. Yang, J., **Zhang, W.**, Meisner, Gregory P., and Chen, L., “Potassium and Sodium Filled Skutterudites”, 20100111754, May 6, 2010.

2. Yang, J., Shi, X., Bai, S., **Zhang, W.**, and Chen, L., “Thermoelectric Material including a Filled Skutterudite Crystal Structure”, 20100071741, March 25, 2010.

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8. L.D. Chen, L. He, X.Y. Huang, R.H. Liu, P.F. Qiu, X. Shi, J. Yang, **W. Zhang**, “Skutterudite thermoelectric material of hole-compensated type and method of making the same”, PCT国际, WO 2013/009430 A1

7. L.D. Chen, Monika, L. He, X.Y. Huang, R.H. Liu, P.F. Qiu, J. Yang, **W. Zhang**, “P-type skutterudite material and method of making the same”, PCT国际, WO2012/024120 A1

6. L.D. Chen, R.H. Liu, P.F. Qiu, **W. Zhang**, X.Y. Huang, X. Shi, J. Yang, L. He, et al., “P-type skutterudite material and method of making the same”, (Korean Patent Application), KR10-2013-7007032, March, 2013

5. L.D. Chen, R.H. Liu, P.F. Qiu, **W. Zhang**, X.Y. Huang, X. Shi, J. Yang, L. He, et al., “P-type skutterudite material and method of making the same”, (Japanese Patent Application), 2013-525938, Feb, 2013

4. L.D. Chen, R.H. Liu, P.F. Qiu, **W. Zhang**, X.Y. Huang, X. Shi, J. Yang, L. He, et al., “P-type skutterudite material and method of making the same”, US13/816829, Aug. 2013

3. L.D. Chen, P.F. Qiu, R.H. Liu, **W. Zhang**, X.Y. Huang, X. Shi, J. Yang, et al., High-Efficiency p-type Skuterudites, China patent, 201110194902.X, 陈立东、仇鹏飞、刘睿恒、张文清、黄向阳、史迅、杨炯、莫尼卡·拜克浩斯，空穴补偿型方钴矿热电材料及其制备方法，中国发明专利(Chinese Patent Application)，201110194902.X

2. Yang, J., Chen, L., Yang, J., Wang, S., **Zhang, W.**, " High Efficiency p-type Skutterudite Compounds", June, 2012.

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##### RESEARCH GRANTS

1. Title: Functional Units and Construction Rules for Non-Semiconductor Thermoelectric Materials

Agency: NSFC key project（基金委重点, 南方科大&上海大学&武汉理工）

Amount: 3,330,000 Yuan

Duration: Jan. 2022 – Dec. 2026

Role: Principal Investigator

1. Title: Multi-scale integrated computing algorithms and software for functional materials in a high-throughput automated process

Agency: Ministry of Science and Technology key project (科技部重点专项)

Amount: 16,125,000 Yuan

Duration: 2017.07-2021.06

Role: Principal Investigator

1. Title: Sub-lattice Engineering and Design for High-efficiency thermoelectrics

Agency: NSFC key project（基金委重点, 上海大学&南方科大）

Amount: 2,850,000 Yuan

Duration: Jan. 2017 – Dec. 2021

Role: Principal Investigator

1. Title: Design principles and realization of novel thermoelectric materials with exotic electrical/thermal transport phenomena

Agency: National Basic Research Program of China (973 子课题)

Amount: 6,000,000 Yuan

Duration: Jan. 2013 – Dec. 2017

Role: Co-Principal Investigator

1. Title: High-efficiency thermoelectric compounds with electron-crystal-phonon-glass characteristics

Agency: NSFC key project（基金委重点，上海硅酸盐所&宁波材料所）

Amount: 3,100,000 Yuan

Duration: Jan. 2013 – Dec. 2017

Role: Principal Investigator

1. Title: Lattice dynamics and thermal conductivity in complex compounds with hierarchy chemical bonds

Agency: NSFC grant（基金委面上）

Amount: 640,000 Yuan

Duration: Jan. 2015 – Dec. 2019

Role: Principal Investigator

1. Title: Program of Shanghai Subject Chief Scientist

Agency: Shanghai Science and Technology Committee（上海市科委）

Amount: 400,000 Yuan

Duration: May. 2016 – Apr. 2019

Role: Principal Investigator

1. Title: High-efficiency Nanostructured Thermoelectric Materials

Agency: NSFC key project under A3 foresight program (China-Japan-Korea A3 international cooperation project，基金委重大国际合作)

Amount: 1,200,000 Yuan

Duration: Jan. 2008 – Dec. 2012

Role: Principal Investigator

1. Title: Computational Materials Science and multiscale design for energy conversion materials

Agency: NSFC special grant for exceptional young scientist（杰出青年基金）

Amount: 2,000,000 Yuan

Duration: Jan. 2008 – Dec. 2012

Role: Principal Investigator

1. Title: Research on Advanced Energy-conversion Materials

Agency: NSFC Innovative Team Project

Amount: 6,000,000 Yuan

Duration: Phase I: Jan. 2008 – Dec. 2011, Phase II: Jan. 2012 – Dec. 2014

Role: Co-Principal Investigator

1. Title: Electrical/Thermal Transport Fundamentals and Design Principles for Novel Thermoelectric Materials

Agency: National Basic Research Program of China (973 子课题)

Amount: 5,000,000 Yuan

Duration: Jan. 2007 –Aug. 2011

Role: Co-Principal Investigator

1. Title: Ab initio Study on the Thermoelectric Properties of Multi-filled CoSb3

Agency: NSFC grant

Amount: 300,000 Yuan

Duration: Jan. 2007 –Dec. 2009

Role: Principal Investigator

1. Title: Methodology Development of Electronic Structure and Transport Property Calculations for Correlated Systems -Electrical Transport Property of hermoelectric Compounds

Agency: NSFC key project

Amount: 2,100,000 Yuan

Duration: Jan. 2007 –Dec. 2010

Role: Co-Principal Investigator

1. Title: Novel Materials with Exotic functions-Thermoelectric Compounds

Agency: CAS knowledge-innovation exploratory project, Novel Materials with Exotic functions-Thermoelectric Compounds

Amount: 1,200,000 Yuan

Duration: Jan. 2010 –Dec. 2012

Role: Co-Principal Investigator

1. Title: Computational Materials Science

Agency: CAS knowledge-innovation exploratory project

Amount: 1,800,000 Yuan

Duration: Jan. 2007 –Dec. 2009

Role: Co-Principal Investigator

1. Title: Computational Materials Physics

Agency: CAS One-hundred-talent plan (百人计划)

Amount: 2,000,000 Yuan

Duration: Jan. 2004 –Aug. 2008

Role: Principal Investigator

1. Title: Ab initio Study on the Adhesion Property of Metal-ceramic Interfaces

Agency: NSFC grant

Amount: 240,000 Yuan

Duration: Jan. 2005 –Dec. 2007

Role: Principal Investigator

1. Title: Research on Advanced Thermoelectric Materials

Agency: International Cooperation Projects, General Motors R&D

Amount: US $ 30,000 /Year

Duration: Jan. 2007 –Dec. 2011

Role: Principal Investigator

1. Title: Research on Advanced Composite Thermoelectric Materials with Effective Phonon Scatters

Agency: International Cooperation Projects, US Corning R&D

Amount: US $ 100,000/year

Duration: Jan. 2007 –Dec. 2012

Role: Co-Principal Investigator

1. Title: Research on multi-dimensional functional motifs and sequence structure and transformative thermoelectric materials

Agency: NSFC key project

Amount: 3,300,000 Yuan

Duration: Jan. 2022 –Dec. 2025

Role: Principal Investigator

1. Title: New material design platform for high-throughput computing and data fusion

Agency: Department of Science and Technology of Guangdong Provincial

Amount: 1,100,000 Yuan

Duration: Jan. 2019 –Dec. 2021

Role: Principal Investigator

1. Title: Electronic-phonon transport physical and thermal functional materials design and application team

Agency: Department of Science and Technology of Guangdong Provincial

Amount: 20,000,000 Yuan

Duration: Sep. 2018 –Sep. 2023

Role: Principal Investigator

1. Title: Study on the electrothermal cooperative transport mechanism and composite thermoelectric material at the base 20180053 interface

Agency: Shenzhen Science and Technology Committee

Amount: 2,000,000 Yuan

Duration: Mar. 2019 –Jan. 2022

Role: Principal Investigator