Yongqing Cai 蔡永青

CONTACT INFORMATION

N23-3004, Institute of Applied Physics and Materials Engineering, University of Macau, Macau, China

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APPOINTMENTS

Assistant Professor, September 2019 – now
Institute of Applied Physics and Materials Engineering,
University of Macau, Macau, China

Scientist III, March 2019 – August 2019
Scientist II, March 2016 – February 2019
Scientist I, January 2013 – February 2016
Institute of High Performance Computing, A*STAR, Singapore

Research Fellow, March 2012 – December 2012
Research Associate, August 2011 – February 2012
Department of Physics, National University of Singapore, Singapore

EDUCATION

Ph.D in Physics, August 2007 - February 2012
National University of Singapore, Singapore
PHD thesis：*First-principles Simulations of Nanomaterials for Nanoelectronics and Spintronics*

M.S. in Materials science, September 2004 - April 2007
Northwestern Polytechnic University, China

B.S. in Materials science, September 2000 - July 2004
Northwestern Polytechnic University, China

TEACHING

GREEN ENERGY FOR GLOBAL SOCIETY (GEGA1006), Undergraduate, University of Macau, Spring semester (2020, 2021, 2022), Fall Semester (2020);
LOW-DIMENSIONAL PHYSICS (APAC3007), Undergraduate, University of Macau, Fall Semester (2021, 2022).
THEORY AND MODELING OF MATERIALS PROPERTIES (APAC4009), Undergraduate, University of Macau, Spring Semester (2023).

HONORS & AWARDS

2020 The National Science Fund for Excellent Young Scholars (Hong Kong & Macau), China
2014 Institute Best Paper Award, Institute of High Performance Computing, A*STAR, Singapore
2007 Distinguished Master Thesis, Northwestern Polytechnic University, China
2004 Distinguished Bachelor Thesis, Faculty of Materials, Northwestern Polytechnic University
2002 1st level, Advanced Mathematics Competition, Shaanxi Province, China

RESEARCH INTERESTS

Computational materials science and physics via first-principles quantum simulations, some more specific area include:

- Phonons: Transport of phonons; Electron-phonon coupling; Raman intensity;

- Phase transition: Ferroelectricity and Multiferroics;
- Light-matter interaction, Polariton;
- Defects: Donors and acceptors; Vacancy clustering; Grain boundary; Twinning
- Artificial intelligence and materials informatics
- Theoretical routes for designing next-generation electronic devices and energy applications

GRANTS

1. Project title: *First-principles Simulations of Two-Dimensional Materials for Nanoelectronics and Energy Harvesting*; Funding Agency: University of Macau (SRG); Principle Investigator; 2019/09/15-2022/09/14;
2. Project title: *Atomic-scale Mechanisms and Efficient Modulation of Layered Transition Metal Chalcogenides for Nanoelectronics*; Funding Agency: The Science and Technology Development Fund (FDCT)-Macau SAR; Principle Investigator; 2020/05/23-2023/05/22;
3. Project title: *High-throughput Materials Informatics*; Funding Agency: National Natural Science Foundation of China (NSFC); Principle Investigator; 2021/01/01-2023/12/31;
4. Project title: *Thermodynamics and Electronic Excitations of Layered Transition Metal Chalcogenides for Layered Transition Metal Chalcogenides*; Funding Agency: Guangdong Research Grant; Principle Investigator; 2021/01/01-2023/12/31;
5. Project title: *Exploration of Exotic Electronic Properties of Novel Two-dimensional Materials*, Funding Agency: University of Macau; Principle Investigator; 2022/01/01-2023/12/31.

SERVICE & PROFESSIONAL ACTIVITY

1. 07/03/2023, Pedagogic Activity, Scientific Talk at Escola Choi Nong Chi Tai (澳門菜農子弟學校)
2. 01/01/2023-now, Associate Editor, Computer Modeling in Engineering & Science (CMES)
3. 20/12/2022, Expert Committee Members, Global Youth Technology and Innovation Forum
4. 16/12/2022, Pedagogic Activity, Scientific Talk at Sacred Heart Canossian College (澳門嘉諾撒聖心女子中學)
5. 01/09/2022-now, Committee Member, Chinese Chemistry Society (Theoretical Chemistry Division) 中國化學學會-理論化學專業委員會成員會委員;
6. 14/10/2021-now, Editorial Board Members, Data;
7. 31/03/2021, Guest Editor, Special Issue for 60th Anniversary Celebration, “Modelling of Low-dimensional Functional Nanomaterials”, *Physica Status Solidi (RRL) - Rapid Research Letters;*
8. 12/03/2021, Pedagogic Activity, Scientific Talk at Yuet Wah College (澳門粵華中學) for whole college student;
9. 02/2021-now, European Materials Modelling Council (EMMC), Associated Member;
10. 16/12/2020, Pedagogic Activity, Tutorial at Cheong Kun Lun College;
11. 14/12/2020, Pedagogic Activity, Scientific Talk at Yuet Wah College (澳門粵華中學) for graduating students

PUBLICATIONS

1 Book
1 Nature Materials, 1 Nature Catalysis, 1 Nature Electronics,
2 Proceedings of the National Academy of Sciences, 4 Nature Communications,
5 Journal of the American Chemical Society, 2 ACS Nano
5 Advanced Materials, 4 Advanced Functional Materials,

10 Physical Review B

Web of Science (publons) : https://www.webofscience.com/wos/author/record/324011
Google Scholar:
https://scholar.google.com.sg/citations?user=902XZNwAAAAJ&hl=zh-CN&oi=ao

Citations	Pablons (Web of Science)	Google scholar
Total	8500	11030
h-index	48	52
i10-index	94	109

*CORRESPONDING AUTHOR
†EQUAL CONTRIBUTION

BOOK:

Yongqing Cai (editor), Gang Zhang, Yong-Wei Zhang, "*Phosphorene: Physical Properties, Synthesis, and Fabrication*", Pan Stanford Publishing, ISBN 9789814774642 (2018).

REPRESENTATIVE PAPERS:

1. Zheng Shu, Hongfei Chen, Xing Liu, Huaxian Jia, Hejin Yan, **Yongqing Cai***, *High-throughput screening of heterogeneous transition metal dual-atom catalysts by synergistic effect for nitrate reduction to ammonia*. **Adv. Funct. Mater.** 2301493 (2023)
2. Tingting Yin*, Hejin Yan, Ibrahim Abdelwahab, Yulia Lekina, Xujie Lü, Wenge Yang, Handong Sun, Kai Leng, **Yongqing Cai***, Ze Xiang Shen*, Kian Ping Loh*, *Pressure driven rotational isomerism in 2D hybrid perovskites*. **Nature Commu.** 14, 411 (2023)
3. Yan Shao, Wei Gao, Hejin Yan, Runlai Li, Ibrahim Abdelwahab, Xiao Chi, Lukas Rogée, Lyuchao Zhuang, Wei Fu, Shu Ping Lau, Siu Fung Yu*, **Yongqing Cai***, Kian Ping Loh*, and Kai Leng*, *Unlocking surface octahedral tilt in two-dimensional Ruddlesden-Popper perovskites*. **Nature Commun.** 13, 138 (2022)
4. Devesh R. Kripalani, **Yongqing Cai***, Jun Lou, and Kun Zhou*, *Strong edge stress in molecularly thin organic–inorganic hybrid Ruddlesden–Popper perovskites and modulations of their edge electronic properties*. **ACS Nano** 16, 1, 261–270 (2022)
5. Jiaren Yuan, Yuanping Chen, Yuee Xie, Xiaoyu Zhang, Dewei Rao, Yandong Guo, Xiaohong Yan*, Yuan Ping Feng*, and **Yongqing Cai***, *Squeezed metallic droplet with tunable Kubo gap and charge injection in transition metal dichalcogenides*. **Proc. Natl. Acad. Sci. U S A** 117, 6362-6369 (2020)
6. **Yongqing Cai**, Qingqing Ke, Gang Zhang, Boris I. Yakobson, and Yong-Wei Zhang, *Highly itinerant atomic vacancies in phosphorene*. **J. Am. Chem. Soc.** 138, 10199-10206 (2016)
7. **Yongqing Cai**, Qingqing Ke, Gang Zhang, Yuan Ping Feng, Vivek B. Shenoy, and Yong-Wei Zhang, *Giant phononic anisotropy and unusual anharmonicity of phosphorene: Interlayer coupling and strain engineering*. **Adv. Funct. Mater.** 25, 2230-2236 (2015) **(Selected as journal Cover)**
8. **Yongqing Cai**, Gang Zhang, Yong-Wei Zhang, Polarity-reversed robust carrier mobility in monolayer MoS_2 nanoribbons. **J. Am. Chem. Soc.** 136, 6269−6275 (2014) **(Highly Cited Paper in Chemistry according to ISI)**

PAPERS:

1. Prem Jyoti Singh Rana, Benny Febriansyah, Teck Ming Koh, Anil Kanwat, Junmin Xia,Teddy Salim, Thomas J. N. Hooper, Mikhail Kovalev, David Giovanni, Yeow Chong Aw,Bhumika Chaudhary, **Yongqing Cai**, Guichuan Xing, Tze Chien Sum, Joel W. Ager, Subodh G. Mhaisalkar, and Nripan Mathews, *Molecular locking with all-organic surface*

modifiers enables stable and efficient slot-die coated methyl-ammonium-free perovskite solar modules, **Adv. Mater.** 2210176 (2023)

2. Xuefei Yan, Xiangyue Cui, Bowen Wang, Hejin Yan, **Yongqing Cai***, Qingqing Ke*, *Surface asymmetry induced turn-overed lifetime of acoustic phonons in monolayer MoSSe*. **iScience**, accepted (2023)
3. Bingtao Liu, Hanxi Sun, Changmeng Huan, Renxu Jia, Yongqing Cai, Qingqing Ke*, *Investigating the reliability of a negative capacitance field effect transistor regarding the electric field across the oxide layer.* **J. Electron. Mater.** 52, 3180–3187 (2023)
4. Zheng Shu, Hongfei Chen, Xing Liu, Huaxian Jia, Hejin Yan, **Yongqing Cai***, *High-throughput screening of heterogeneous transition metal dual-atom catalysts by synergistic effect for nitrate reduction to ammonia*. **Adv. Funct. Mater.** 2301493 (2023)
5. Zheng Shu, and **Yongqing Cai***, *Thickness-dependent catalytic activity of hydrogen evolution based on single atomic catalyst of Pt above MXene*. **J. Phys.: Condens. Matter** 35, 204001 (2023)
6. Guotao Qiu, Zongjin Li*, Kun Zhou, and **Yongqing Cai***, *Flexomagnetic noncollinear state with a plumb line shape spin configuration in edged two-dimensional magnetic CrI_3.* **npj Quantum Mater.** 8, 15 (2023)
7. Changmeng Huan, **Yongqing Cai***, Devesh R. Kripalani, Kun Zhou, and Qingqing Ke*, *Abnormal behavior of preferred formation of the cationic vacancies from the interior in a γ-GeSe monolayer with the stereo-chemical antibonding lone-pair state*. **Nanoscale Horiz.** 8, 404-411 (2023)
8. Tingting Yin*, Hejin Yan, Ibrahim Abdelwahab, Yulia Lekina, Xujie Lü, Wenge Yang, Handong Sun, Kai Leng, **Yongqing Cai***, Ze Xiang Shen*, and Kian Ping Loh*, *Pressure driven rotational isomerism in 2D hybrid perovskites*. **Nat. Commu.** 14, 411 (2023)
9. Xing Ming*, Qing Liu*, Miaomiao Wang*, **Yongqing Cai***, Binmeng Chen*, and Zongjin Li*, *Improved chloride binding capacity and corrosion protection of cement-based materials by incorporating alumina nano particles*. **Cem. Concr. Compos.** 136, 104898 (2023)
10. Xing Ming*, Yunjian Li*, Qing Liu*, Miaomiao Wang*, **Yongqing Cai***, Binmeng Chen*, and Zongjin Li*, *Chloride binding behaviors and early age hydration of tricalcium aluminate in chloride-containing solutions*. **Cem. Concr. Compos.** 137, 104928 (2023)
11. Ruxin Guo, Junmin Xia, Hao Gu, Xuke Chu, Yan Zhao, Xianghuan Meng, Zhiheng Wu, Jiangning Li, Yanyan Duan, Zhenzhen Li, Zhaorui Wen, Shi Chen, **Yongqing Cai**, Chao Liang, Yonglong Shen, Guichuan Xing, Wei Zhang, and Guosheng Shao, *Effective defect passivation with a designer ionic molecule for high-efficiency vapour-deposited inorganic phase-pure $CsPbBr_3$ perovskite solar cells*. **J. Mater. Chem. A** 11, 408-418 (2023)
12. Yu-Long Hai, He-Jin Yan, and **Yong-Qing Cai***, *Structural screening of phosphorus sulfur ternary hydride PSH6 with a high-temperature superconductivity at 130 Gpa*. **Front. Phys.** 18, 23303 (2023)
13. Zheng Shu, Bowen Wang, Xiangyue Cui, Xuefei Yan, Hejin Yan, Huaxian Jia, **Yongqing Cai***, *High-performance thermoelectric monolayer γ-GeSe and its group-IV monochalcogenide isostructural family.* **Chem. Eng. J.** 454, 140242 (2023)
14. Xiangyue Cui, Xuefei Yan, Bowen Wang, and **Yongqing Cai***, *Phononic transport in 1T′-$MoTe_2$: Anisotropic structure with an isotropic lattice thermal conductivity*. **Appl. Surf. Sci.** 608, 155238 (2023)
15. Kangdi Niu, Guotao Qiu, Chuanshou Wang, Daiyue Li, Yutao Niu, Songge Li, Lixing Kang, **Yongqing Cai***, Mengjiao Han*, Junhao Lin*, *Self-intercalated magnetic heterostructures in 2D chromium telluride*. **Adv. Funct. Mater.** DOI: 10.1002/adfm.202208528 (2022)
16. Ziqing Ye, Junmin Xia, Dengliang Zhang, Xingxing Duan, Zhaohui Xing, Guangrong Jin, **Yongqing Cai**, Guichuan Xing, Jiangshan Chen, Dongge Ma, *Efficient quasi-2D perovskite*

light-emitting diodes enabled by regulating phase distribution with a fluorinated organic cation. **Nanomaterials** 12, 3495 (2022)

17. Qiye Guan, Hejin Yan, and **Yongqing Cai***, *Strongly modulated exfoliation and functionalization of MXenes with rationally designed groups in polymer: A Theoretical Study.* **Chem. Mater.** 34, 9414 (2022)
18. Bowen Wang, Xuefei Yan, Xiangyue Cui, and **Yongqing Cai***, *First-principles study of the phonon lifetime and low lattice thermal conductivity of monolayer γ-GeSe: A comparative study.* **ACS Appl. Nano Mater.** 5, 15441–15448 (2022)
19. Xuefei Yan, Bowen Wang, Yulong Hai, Devesh R. Kripalani, Qingqing Ke, and **Yongqing Cai***, *Phonon anharmonicity and thermal conductivity of two-dimensional van der Waals materials: A review*. **Sci. China: Phys. Mech. Astron.** 65, 117004 (2022)
20. Hejin Yan, Qiye Guan, Hongfei Chen, Xiangyue Cui, Zheng Shu, Dan Liang, Bowen Wang and **Yongqing Cai***, *Low-energy intralayer phonon assisted carrier recombination in Z-scheme van der Waals heterostructures for photocatalysis*. **J. Mater. Chem. A** 10, 23744 - 23750 (2022)
21. Xing Ming, Qing Liu, Yunjian Li, **Yongqing Cai***, and Zongjin Li*, *Ab-initio modeling of chloride binding at hydrocalumite/sodium chloride solution interfaces*. **Cem. Concr. Res.** 162, 106996 (2022)
22. Xing Ming, **Yongqing Cai***, and Zongjin Li*, *Atomic scale insight into the mechanisms of chloride induced steel corrosion in concrete.* **Constr Build Mater.** 351, 128811 (2022)
23. Zheng Shu, Xiangyue Cui, Bowen Wang, Hejin Yan, and **Yongqing Cai***, *Fast Intercalation of Lithium in Semi-Metallic γ-GeSe Nanosheet: A New Group-IV Monochalcogenide for Lithium-Ion Battery Application*. **ChemSusChem,** 15, e202200564 (2022)
24. Junmin Xia, Chao Liang*, Hao Gu, Shiliang Mei, Shengwen Li, Nan Zhang, Shi Chen, **Yongqing Cai***, and Guichuan Xing*, *Surface passivation towards efficient and stable perovskite solar cells.* **Energy Environ. Mater.** 10.1002/eem2.12296 (2022)
25. Jiajun Feng, Hongmin Liu, Zhe Ma, Jiahao Feng, Lianfen Chen, Junhao Li, **Yongqing Cai**, Qingguang Zeng, Dawei Wen, Yue Guo, *A super stable near-infrared garnet phosphor resistant to thermal quenching, thermal degradation and hydrolysis*. **Chem. Eng. J.** 449, 137892 (2022)
26. Yuanxia Li, Jingxin Zhao*, Qiang Hu, Tianwei Hao, Heng Cao, Xiaomin Huang, Yu Liu, Yanyan Zhang, Dunmin Lin*, Yuxin Tang*, **Yongqing Cai***, *Prussian blue analogs cathodes for aqueous zinc ion batteries*. **Mater. Today Energy** 29, 101095 (2022).
27. Xiaozong Hu, Kailang Liu, **Yongqing Cai**, Shuang-Quan Zang, Tianyou Zhai, *2D Oxides for Electronics and Optoelectronics*. **Small Science** 2, 2200008 (2022)
28. Changmeng Huan, Pu Wang, Binghan He, **Yongqing Cai***, and Qingqing Ke*, *Highly modulated dual semimetal and semiconducting γ-GeSe with strain engineering*. **2D Materials** 9 045014 (2022)
29. Changmeng Huan, Pu Wang, Bingtao Liu, Binghan He, **Yongqing Cai***, and Qingqing Ke*, *Versatile van der Waals heterostructures of γ-GeSe with h-BN/graphene/MoS_2.* **J. Mater. Chem. C** 10, 10995-11004 (2022)
30. Jiaren Yuan, Qingyuan Wei, Minglei Sun, Xiaohong Yan, **Yongqing Cai***, Lei Shen*, and Udo Schwingenschlögl, *Protected valley states and generation of valley- and spin-polarized current in monolayer MA_2Z_4*. **Phys. Rev. B** 105, 195151 (2022)
31. Hao Gu, Tingting Niu, Shouwei Zuo, **Yongqing Cai**, Lingfeng Chao, Peter Müller-Buschbaum, Yingdong Xia, Jing Zhang, Guichuan Xing, and Yonghua Chen, *Stable metal halide perovskite colloids in protic ionic liquid*. **CCS Chemistry**, 10.31635/ccschem.022.202101629, 1-24 (2022)
32. Junmin Xia, Hao Gu, Chao Liang, **Yongqing Cai***, and Guichuan Xing*, *Manipulation of*

band alignment in two-dimensional vertical WSe2/BA2PbI4 Ruddlesden–Popper perovskite heterojunctions via defect engineering. **J. Phys. Chem. Lett.** 13, 4579–4588 (2022)

33. Hejin Yan, Bowen Wang, Xuefei Yan, Qiye Guan, Hongfei Chen, Zheng Shu, Dawei Wen, and **Yongqing Cai***, *Efficient passivation of surface defects by Lewis base in lead-free tin-based perovskite solar cells.* **Mater. Today Energy** 27, 101038 (2022)
34. Dan Liang, Shi Xu, Pengfei Lu*, and **Yongqing Cai***, *Highly tunable and strongly bound exciton in $MoSi_2N_4$ via strain engineering*. **Phys. Rev. B** 105, 195302 (2022)
35. Hanyan Fang, Aurelio Gallardo, Dikshant Dulal, Zhizhan Qiu, Jie Su, Mykola Telychko, Harshitra Mahalingam, Pin Lyu, Yixuan Han, Yi Zheng, **Yongqing Cai**, Aleksandr Rodin, Pavel Jelínek, and Jiong Lu, *Electronic self-passivation of single vacancy in black phosphorus via ionization*. **Phys. Rev. Lett.** 128, 176801 (2022)
36. Junmin Xia, Chao Liang, Hao Gu, Shiliang Mei, **Yongqing Cai***, and Guichuan Xing*, *Two-dimensional heterostructure of MoS_2/BA_2PbI_4 2D Ruddlesden–Popper perovskite with an S Scheme alignment for solar cells: A first-principles study*. **ACS Appl. Electron. Mater.** 4, 1939–1948 (2022)
37. Bowen Wang, Xuefei Yan, Hejin Yan, **Yongqing Cai***, *Strong reduction of thermal conductivity of WSe_2 with introduction of atomic defects*. **Nanotechnology** 33, 275706 (2022)
38. Guotao Qiu, **Yongqing Cai***, Zongjin Li*, *Multiscale investigation of magnetic field distortion on surface of ferromagnetic materials caused by stress concentration for metal magnetic memory method*. **Comput. Mater. Sci.** 209, 111353 (2022)
39. Bowen Wang, Xuefei Yan, Hejin Yan, **Yongqing Cai***, *Size and stoichiometric dependence of thermal conductivities of InxGa1-xN: A molecular dynamics study.* **Comput. Mater. Sci.** 207, 111321 (2022)
40. Xuefei Yan, Qingqing Ke* and **Yongqing Cai***, *Electronic and optical properties of Janus black arsenic-phosphorus AsP quantum dots under magnetic field.* **Nanotechnology** 33, 265001 (2022)
41. Kun Zhou*, Bo Liu*, **Yongqing Cai***, Sergey V. Dmitriev*, Shaofan Li*, *Modelling of low-dimensional functional nanomaterials*. **Phys. Status Solidi RRL** 16, 2100654 (2022)
42. Zheng Shu, Hejin Yan, Hongfei Chen, **Yongqing Cai***, *Mutual modulation via charge transfer and unpaired electrons of catalytic sites for the superior intrinsic activity of N_2 reduction: from high-throughput computation assisted with a machine learning perspective*. **J. Mater. Chem. A** 10, 5470-5478 (2022)
43. Qingyuan Wei, Dongke Chen, **Yongqing Cai**, Lei Shen, Jing Xu, Jiaren Yuan, Yuanping Chen, Xiaohong Yan, *Generation and enhancement of valley polarization in monolayer chromium dichalcogenides*. **J. Supercond. Nov. Magn.** 35, 787–794 (2022)
44. Qiye Guan, Hejin Yan, and **Yongqing Cai***, *Flatten the Li-ion activation in perfectly lattice-matched MXene and 1T-MoS_2 heterostructures via chemical functionalization*, **Adv. Mater. Interfaces**. 2101838 (2022)
45. Hongfei Chen, Hejin Yan, and **Yongqing Cai***, *Effects of defect on work function and energy alignment of PbI_2: Implications for solar cell applications*. **Chem. Mater.** 34, 1020–1029 (2022)
46. Changmeng Huan, Wang Pu, Binghan He, **Yongqing Cai***, and Qingqing Ke*, *Oxygen deficient α-MoO_3 with promoted adsorption and state-quenching of H_2O for gas sensor: A DFT Study*. **J. Mater. Chem. C** 10, 1839-1849 (2022)
47. Devesh R. Kripalani, **Yongqing Cai***, Jun Lou, and Kun Zhou*, *Strong edge stress in molecularly thin organic–inorganic hybrid Ruddlesden–Popper perovskites and modulations of their edge electronic properties*. **ACS Nano** 16, 1, 261–270 (2022)
48. Yan Shao, Wei Gao, Hejin Yan, Runlai Li, Ibrahim Abdelwahab, Xiao Chi, Lukas Rogée,

Lyuchao Zhuang, Wei Fu, Shu Ping Lau, Siu Fung Yu*, **Yongqing Cai***, Kian Ping Loh*, and Kai Leng*, *Unlocking surface octahedral tilt in two-dimensional Ruddlesden-Popper perovskites*. **Nature Commun.** 13, 138 (2022)

49. Junmin Xia, Chao Liang*, Hao Gu, Shiliang Mei, Shengwen Li, Nan Zhang, Shi Chen, **Yongqing Cai***, and Guichuan Xing*, *Surface passivation towards efficient and stable perovskite solar cells.* **Energy Environ. Mater.** 10.1002/eem2.12296 (2022)
50. Zheng Shu, and **Yongqing Cai***, *Activation of phosphorene-like two-dimensional GeSe for efficient electrocatalytic nitrogen reduction via states filtering of Ru*. **J. Mater. Chem. A** 9, 16056-16064 (2021)
51. Ying Zhang, Lixun Xue, Chenbin Liang, Yizhuang Chen, Junjie Liu, Chuang Shen, Qi Li, Yefan Duan, Liyuan Yao, Hao Zhang, **Yongqing Cai***, Chaoliang Tan*, Zhimin Luo*, *Two-dimensional metallic MoS_2-amorphous $CoNi(OH)_2$ nanocomposite for enhanced electrochemical water splitting in alkaline solutions*. **Appl. Surf. Sci.** 561, 150079 (2021)
52. Xinke Liu, Shengqun Hu, Jiangliu Luo, Xiaohua Li*, Jing Wu, Dongzhi Chi, Kah-Wee Ang, Wenjie Yu, **Yongqing Cai***, *Suspended MoS_2 photodetector using patterned sapphire substrate*. **Small**, 2100246 (2021)
53. Junmin Xia, Chao Liang, Shiliang Mei, Hao Gu, Bingchen He, Zhipeng Zhang, Tanghao Liu, Kaiyang Wang, Sisi Wang, Shi Chen, **Yongqing Cai***, and Guichuan Xing*, *Deep surface passivation for efficient and hydrophobic perovskite solar cells*. **J. Mater. Chem. A**, 9, 2919-2927 (2021)
54. Fenfa Yao†, **Yongqing Cai**†, Zhangru Xiao, Gang Zhang, Rong-Jun Xie, and Chuanhong Jin, *In situ transmission electron microscopy study of the formation and migration of vacancy defects in atomically thin black phosphorus*. **2D Mater.** 8, 025004 (2021)
55. Zhun-Yong Ong, **Yongqing Cai**, Gang Zhang, and Yong-wei Zhang, *Theoretical analysis of thermal boundary conductance of MoS_2-SiO_2 and WS_2-SiO_2 interface*. **Nanotechnology** 32, 135402 (2021)
56. Kai Leng, Lin Wang, Yan Shao, Ibrahim Abdelwahab, Gustavo Grinblat, Ivan Verzhbitskiy, Runlai Li, **Yongqing Cai**, Xiao Chi, Wei Fu, Peng Song, Andrivo Rusydi, Goki Eda, Stefan A. Maier, and Kian Ping Loh, *Electron tunneling at the molecularly thin 2D perovskite and graphene van der Waals interface*. **Nature Commun.** 11, 5483 (2020)
57. Zheng Shu, and **Yongqing Cai***, *Substitutional doped GeSe: tunable oxidative states with strain engineering*. **J. Mater. Chem. C** 8, 13655-13667 (2020)
58. Kai Ren, Wencheng Tang, Minglei Sun, **Yongqing Cai**, Yuan Cheng, and Gang Zhang, *A direct Z-scheme PtS_2/arsenene van der Waals heterostructure with high photocatalytic water splitting efficiency.* **Nanoscale** 12, 17281-17289 (2020)
59. Jing Wu, Yanpeng Liu, Yi Liu, **Yongqing Cai**, Yunshan Zhao, Hong Kuan Ng, Kenji Watanabe, Takashi Taniguchi, Gang Zhang, Cheng-Wei Qiu, Dongzhi Chi, A. H. Castro Neto, John T. L. Thong, Kian Ping Loh, and Kedar Hippalgaonkar, *Large enhancement of thermoelectric performance in MoS_2/h-BN heterostructure due to vacancy-induced band hybridization*. **Proc. Natl. Acad. Sci. U S A** 117, 13929-13936 (2020)
60. Jiaren Yuan, Yuanping Chen, Yuee Xie, Xiaoyu Zhang, Dewei Rao, Yandong Guo, Xiaohong Yan*, Yuan Ping Feng*, and **Yongqing Cai***, *Squeezed metallic droplet with tunable Kubo gap and charge injection in transition metal dichalcogenides*. **Proc. Natl. Acad. Sci. U S A** 117, 6362-6369 (2020)
61. Jiaren Yuan, Yumeng Yang, **Yongqing Cai**, Yihong Wu, Yuanping Chen, Xiaohong Yan, and Lei Shen, *Intrinsic skyrmions in monolayer Janus magnets*. **Phys. Rev. B** 101, 094420 (2020)
62. Yu Jun Tan, Hareesh Godaba, Ge Chen, Siew Ting Melissa Tan, Guanxiang Wan, Guojingxian Li, Pui Mun Lee, **Yongqing Cai**, Si Li, Robert F. Shepherd, John S. Ho &

Benjamin C. K. Tee, *A transparent, self-healing and high-κ dielectric for low-field-emission stretchable optoelectronics*. **Nature Materials** 19, 182–188 (2020)

63. Devesh R. Kripalani, **Yongqing Cai***, Ming Xue, and Kun Zhou*, *Metastable interlayer Frenkel pair defects in black phosphorus*. **Phys. Rev. B** 100, 224107 (2019)
64. Bin Du†, Qi Wei†, **Yongqing Cai**†, Tanghao Liu, Bo Wu, Ying Li, Yonghua Chen, Yingdong Xia, Guichuan Xing, and Wei Huang, *Crystal face dependent charge carrier extraction in TiO_2/perovskite heterojunctions*. **Nano Energy** 67, 104227 (2019)
65. **Yongqing Cai**, Junfeng Gao, Shuai Chen, Qingqing Ke, Gang Zhang, Yong-Wei Zhang, *Design of phosphorene for hydrogen evolution performance comparable to platinum*. **Chem. Mater.** 31, 8948-8956 (2019)
66. Xing Wu†, **Yongqing Cai**†, Jihong Bian†, Guohui Su, Chen Luo, Yaodong Yang, and Gang Zhang, *Strain engineering and lattice vibration manipulation of atomically thin TaS_2 films*. **RSC Adv.** 10, 16718-16726 (2020)
67. **Yongqing Cai**, Gang Zhang, and Yong-Wei Zhang, *Staggering transport of edge states and symmetry analysis of electronic and optical properties of stanene*. **Nanoscale** 12, 20890-20897 (2020)
68. Fen Qiao*, Rong Kang, Qichao Liang, **Yongqing Cai***, Jiming Bian, and Xiaoya Hou. *Tunability in the optical and electronic properties of ZnSe microspheres via Ag and Mn doping*. **ACS omega** 4, 12271-12277 (2019)
69. **Yongqing Cai**, Shuai Chen, Junfeng Gao, Gang Zhang, and Yong-Wei Zhang. *Evolution of intrinsic vacancies and prolonged lifetime of vacancy clusters in black phosphorene.* **Nanoscale** 11, 20987-20995 (2019)
70. Yunshan Zhao, **Yongqing Cai**, Lifa Zhang, Baowen Li, Gang Zhang, John TL Thong. *Thermal transport in 2D semiconductors—considerations for device applications*. **Adv. Funct. Mater.** 1903929 (2019)
71. Yue Cao, Yu Jun Tan, Si Li, Wang Wei Lee, Hongchen Guo, **Yongqing Cai**, Chao Wang, Benjamin C.-K. Tee, *Self-healing electronic skins for aquatic environments*. **Nature Electronics** 2, 75–82 (2019)
72. Qingqing Ke, Zhang Xiao, Zang Wenjie, Abdelnaby M. Elshahawy, Yating Hu, Qiyuan He, Stephen J. Pennycook, **Yongqing Cai***, John Wang*, *Strong charge transfer at 2H‐1T phase boundary of MoS_2 for superb high‐performance energy storage*. **Small** 15, 1900131 (2019)
73. Andrey A. Kistanov, Devesh R. Kripalani, **Yongqing Cai***, Sergey V. Dmitriev, Kun Zhou*, and Yong-Wei Zhang*, *Ultrafast diffusive cross-sheet motion of lithium through antimonene with 2 + 1 Dimensional Kinetics*. **J. Mater. Chem. A** 7, 2901-2907 (2019)
74. Fayyaz Hussain, Muhammad Imran, Anwar Manzoor Rana, Muhammad Ismail, R.M. ArifKhalil, M. AtifSattar, M. ArshadJavid, Abdul Majid, **Yongqing Cai**, *Tailoring magnetic characteristics of phosphorene by the doping of Ce and Ti: A DFT study*. **Physica E Low Dimens. Syst. Nanostruct.** 106, 352-356 (2019)
75. Hong Kuan Ng, Anas Abutaha, Damien Voiry, Ivan Verzhbitskiy, **Yongqing Cai**, Gang Zhang, Yi Liu, Jing Wu, Manish Chhowalla, Goki Eda, and Kedar Hippalgaonkar, *Effects of structural phase transition on thermoelectric performance in lithium-intercalated molybdenum disulfide (Li_xMoS_2).* **ACS Appl. Mater. Interfaces** 11, 12184−12189 (2019)
76. Chunlin Zhao, Haijun Wu, Fei Li, **Yongqing Cai**, Yang Zhang, Dongsheng Song, Jiagang Wu, Xiang Lyu, Jie Yin, Dingquan Xiao, Jianguo Zhu, and Stephen J. Pennycook, *Practical high piezoelectricity in barium titanate ceramics utilizing multiphase convergence with broad structural flexibility*. **J. Am. Chem. Soc.** 140, 15252-15260 (2018)
77. Xiao Zhang†, Zhimin Luo†, Peng Yu†, **Yongqing Cai**†, Yonghua Du, Daoxiong Wu, Si Gao, Chaoliang Tan, Zhong Li, Minqin Ren, Thomas Osipowicz, Shuangming Chen, Zheng

Jiang, Jiong Li, Ying Huang, Jian Yang, Ye Chen, Chung Yen Ang, Yanli Zhao, Peng Wang, Li Song, Xiaojun Wu, Zheng Liu, Armando Borgna and Hua Zhang, *Lithiation-induced amorphization of $Pd_3P_2S_8$ for highly efficient hydrogen evolution*. **Nature Catalysis** 1, 460 (2018)

78. Jiaren Yuan[‘], **Yongqing Cai**[†], Lei Shen, Yang Xiao, Ji-Chang Ren, Aizhu Wang, Yuan Ping Feng, Xiaohong Yan, *One-dimensional thermoelectrics induced by Rashba spin-orbit coupling in two-dimensional BiSb monolayer*. **Nano Energy** 52, 163-170 (2018)
79. Devesh R. Kripalani, Andrey A. Kistanov, **Yongqing Cai***, Ming Xue, and Kun Zhou*, *Strain engineering of antimonene by a first-principles study: mechanical and electronic properties*. **Phys. Rev. B** 98, 085410 (2018)
80. Chongling Cheng, **Yongqing Cai**, Guijian Guan, Leslie Yeo, Dayang Wang, *Hydrophobic force-driven removal of organic compounds from water by reduced graphene oxides built in agarose hydrogels*. **Angew. Chem.** 57, 11177-11181 (2018)
81. Guijian Guan, Mingda Wu, **Yongqing Cai**, Shuhua Liu, Yuan Cheng, Si Yin Tee, Yong-Wei Zhang, Ming-Yong Han, *Surface-mediated chemical dissolution of two-dimensional nanomaterials toward hole creation*. **Chem. Mater.** 30, 5108–5115 (2018)
82. Jing Xia, Zhi Li Dong, **Yongqing Cai**, Guijian Guan, Shuangyuan Zhang, András Kovács, Chris Boothroyd, In Yee Phang, Shuhua Liu, Mingda Wu, Yong Wei Zhang, Xiao Hu, Ming-Yong Han, *Morphological growth and theoretical understanding of gold and other noble metal nanoplates*. **Chem-Eur J.** 24, 15589-15595 (2018)
83. Taotao Li, Chaowei Li, **Yongqing Cai**, Junhao Lin, Xiaoyang Long, Liangjie Wang, Yancui Xu, Juan Sun, Lei Tang, Yong-Wei Zhang, Kazu Suenaga, Zheng Liu, Yagang Yao, *Highly efficient mass production of boron nitride nanosheets via a borate nitridation method*. **J. Phys. Chem. C** 122, 17370–17377 (2018)
84. Xin Huang, **Yongqing Cai**, Xuewei Feng, Wee Chong Tan, Dihan Md. Nuruddin Hasan, Li Chen, Nan Chen, Lin Wang, Li Huang, Thorin Jake Duffin, Christian A. Nijhuis, Yong-Wei Zhang, Chengkuo Lee, and Kah-Wee Ang, *Black phosphorus carbide as a tunable anisotropic plasmonic metasurface.* **ACS Photonics** 5, 3116–3123 (2018)
85. Guofeng Xie, Zhifang Ju, Kuikui Zhou, Xiaolin Wei, Zhixin Guo, **Yongqing Cai** and Gang Zhang, *Ultra-low thermal conductivity of two-dimensional phononic crystals in the incoherent regime*. **NPJ Comp. Mater.** 4, 21 (2018)
86. Chaoliang Tan, Zhimin Luo, Apoorva Chaturvedi, **Yongqing Cai**, Yonghua Du, Yue Gong, Ying Huang, Zhuangchai Lai, Xiao Zhang, Lirong Zheng, Xiaoying Qi, Min Hao Goh, Jie Wang, Shikui Han, Xue-Jun Wu, Lin Gu, Christian Kloc, Hua Zhang, *Preparation of high-percentage 1T-phase transition metal dichalcogenide nanodots for electrochemical hydrogen evolution.* **Adv. Mater.** 30, 1705509 (2018)
87. Andrey A. Kistanov, **Yongqing Cai***, Kun Zhou*, Narasimalu Srikanth, Sergey V. Dmitriev and Yong-Wei Zhang*, *Exploring the charge localization and band gap opening of borophene: a first-principles study*. **Nanoscale** 10, 1403-1410 (2018)
88. Andrey A. Kistanov, **Yongqing Cai***, Kun Zhou*, Sergey V. Dmitriev and Yong-Wei Zhang*, *Atomic-scale mechanisms of defect- and light-induced oxidation and degradation of InSe*. **J. Mater. Chem. C** 6, 518-525 (2018)
89. Andrey A. Kistanov, **Yongqing Cai***, Kun Zhou*, Sergey V. Dmitriev, and Yong-Wei Zhang*, *Effects of graphene/BN encapsulation, surface functionalization and molecular adsorption on the electronic properties of layered InSe: a first-principles study*. **Phys. Chem. Chem. Phys.** 20, 12939-12947 (2018)
90. Andrey Kistanov, **Yongqing Cai***, Devesh Kripalani, Kun Zhou*, Sergey Dmitriev, and Yong-Wei Zhang*, *A First-Principles Study on the Adsorption of Small Molecules on Antimonene: Oxidation Tendency and Stability*. **J. Mater. Chem. C** 6, 4308-4317 (2018)

91. Hangbo Zhou, **Yongqing Cai**, Gang Zhang and Yong-Wei Zhang, *Unusual phonon behavior and ultra-low thermal conductance of monolayer InSe*. **Nanoscale** 10, 480-487 (2018)
92. Hongfei Liu, **Yongqing Cai**, Ming-Yong Han, Shifeng Guo, Ming Lin, Meng Zhao, Yong-Wei Zhang, and Dongzhi Chi, *Aqueous and mechanical exfoliation, unique properties and theoretical understanding of MoO_3 nanosheets from free standing α-MoO_3 crystals: Raman mode softening and blueshift in absorption edge*. **Nano Res.** 11, 1193–1203 (2018)
93. Yuan Cheng, Gang Zhang, Yingyan Zhang, Tienchong Chang, Qing-Xiang Pei, **Yongqing Cai** and Yong-Wei Zhang, *Large diffusion anisotropy and orientation sorting of phosphorene nanoflakes under temperature gradient.* **Nanoscale** 10, 1660-1666 (2018)
94. V. Sorkin, **Y. Q. Cai**, D. J. Srolovitz, and Y. W. Zhang, *Mechanical twinning in phosphorene*. **Extreme Mech. Lett.** 19, 15-19 (2018)
95. Subhadeep Datta[†], **Yongqing Cai**[†], Indra Yudhistira, Zebing Zeng, Yong-Wei Zhang, Han Zhang, Shaffique Adam, Jishan Wu, and Kian Ping Loh, *Tuning magnetoresistance in molybdenum disulphide and graphene using a molecular spin transition*. ***Nature Commun.*** 8, 677 (2017)
96. Yifei Yu, Guoqing Li, Lujun Huang, Andrew Barrette, **Yong-Qing Cai**, Yiling Yu, Kenan Gundogdu, Yong-Wei Zhang, and Linyou Cao, *Enhancing multifunctionalities of transition-metal dichalcogenide monolayers via cation intercalation*. **ACS Nano** 11, 9390-9396 (2017)
97. Yating Hu,* Yu Zhang, Du Yuan, Xu Li, **Yongqing Cai*,** and John Wang*, *Controllable structure transitions of Mn_3O_4 nanomaterials and their effects on electrochemical properties*. **Nanoscale Horiz.** 2, 326-332 (2017)
98. Wee Chong Tan, **Yongqing Cai**, Rui Jie Ng, Li Huang, Xuewei Feng, Gang Zhang, Yong-Wei Zhang, Christian A. Nijhuis, Xinke Liu, Kah-Wee Ang, *Few-layer black phosphorus carbide field-effect transistor via carbon doping*. **Adv. Mater.** 29, 1700503 (2017)
99. **Yongqing Cai**, Gang Zhang, and Yong-Wei Zhang, *Charge transfer and functionalization of monolayer InSe by physisorption of small molecules for gas sensing*. **J. Phys. Chem. C** 121,10182–10193 (2017)
100. Andrey A Kistanov, **Yongqing Cai**, Yong-Wei Zhang, Sergey V Dmitriev, and Kun Zhou, *Strain and water effects on the electronic structure and chemical activity of in-plane graphene/silicene heterostructure*. **J. Phys.: Condens. Matter** 29, 095302 (2017)
101. Hangbo Zhou, **Yongqing Cai,** Gang Zhang & Yong-Wei Zhang, *Superior lattice thermal conductance of single-layer borophene*. **NPJ 2D Materials and Applications** 1, 14 (2017)
102. Yuanda Liu, **Yongqing Cai,** Gang Zhang, Yong-Wei Zhang, and Kah-Wee Ang, *Al-doped black phosphorus p–n homojunction diode for high performance photovoltaic*. **Adv. Funct. Mater.** 1604638 (2017)
103. Qingqing Ke, Cao Guan, Xiao Zhang, Minrui Zheng, Yong-Wei Zhang, **Yongqing Cai*,** Hua Zhang*, and John Wang*, *Surface-charge-mediated formation of H-TiO_2@$Ni(OH)_2$ heterostructures for high-performance supercapacitors*. **Adv. Mater.** 29, 1604164 (2017) **(Highly Cited Paper in Materials Science according to ISI)**
104. Andrey A Kistanov, **Yongqing Cai*****, Kun Zhou*****, Sergey V Dmitriev, and Yong-Wei Zhang*****, *The role of H_2O and O_2 molecules and phosphorus vacancies in the structure instability of phosphorene*. **2D Mater.** 4, 015010 (2017)
105. Amit Prakash[†], **Yongqing Cai**[†], Gang Zhang, Yong-Wei Zhang, and Kah-Wee Ang, *Black phosphorus n-type field-effect transistor with ultrahigh electron mobility via aluminum adatoms doping*. **Small** 13, 1602909 (2017)
106. Andrey A Kistanov, **Yongqing Cai**, Kun Zhou, Sergey V. Dmitriev, Narasimalu Srikanth,

Danial Saadatmand, Yong-Wei Zhang, *Strain and Defects Engineering of Phosphorene*, Asian Conference on Energy, Power and Transportation Electrification (ACEPT), Singapore, (2017)

107. **Yongqing Cai***, Yuan Ping Feng*, *Review on charge transfer and chemical activity of TiO_2: Mechanism and applications*. **Prog. Surf. Sci.** 91, 183–202 (2016)
108. **Yongqing Cai**, Hangbo Zhou, Gang Zhang, and Yong-Wei Zhang, *Modulating carrier density and transport properties of MoS_2 by organic molecular doping and defect engineering*. **Chem. Mater.** 28, 8611–8621 (2016)
109. Zhun-Yong Ong, **Yongqing Cai**, and Gang Zhang, *Theory of substrate-directed heat dissipation for single-layer graphene and other two-dimensional crystals*. **Phys. Rev. B** 94, 165427 (2016)
110. Hangbo Zhou, **Yongqing Cai**, Gang Zhang, and Yong-Wei Zhang, *Thermoelectric properties of phosphorene at the nanoscale*. **J. Mater. Res.** 31, 3179-3186 (2016)
111. Hangbo Zhou, **Yongqing Cai**, Gang Zhang, and Yong-Wei Zhang, *Quantum thermal transport in stanene*. **Phys. Rev. B** 94, 045423 (2016)
112. V. Sorkin, **Y. Cai**, Z. Ong, G. Zhang, Y. W. Zhang, *Recent advances in the study of phosphorene and its nanostructures*. **Critical Reviews in Solid State and Materials Sciences**, 1-82 (2016)
113. **Yongqing Cai**, Qingqing Ke, Gang Zhang, Boris I. Yakobson, and Yong-Wei Zhang, *Highly itinerant atomic vacancies in phosphorene*. **J. Am. Chem. Soc.** 138, 10199-10206 (2016)
114. Muhammad Imran, Fayyaz Hussain, Muhammad Rashid, Muhammad Ismail, Hafeez Ullah, **Yongqing Cai**, M Arshad Javid, Ejaz Ahmad, S A Ahmad, *Molecular dynamics simulation of nanoscale surface diffusion of heterogeneous adatoms clusters*. **Chin. Phys. B** 25**,** 076601 (2016)
115. Yifei Yu, Yiling Yu, Chao Xu, **Yong-Qing Cai**, Liqin Su, Yong Zhang, Yong-Wei Zhang, Kenan Gundogdu, Linyou Cao, *Engineering substrate interactions for high luminescence efficiency of transition metal dichalcogenide monolayers*. **Adv. Funct. Mater.** 26**,** 4733–4739 (2016)
116. Andrey Kistanov, **Yongqing Cai***, Kun Zhou*, Sergey Dmitriev, Yong-Wei Zhang, *Large electronic anisotropy and enhanced chemical activity of highly rippled phosphorene*. **J. Phys. Chem. C** 120, 6876–6884 (2016)
117. **Yongqing Cai**, Qing-Xiang Pei, Gang Zhang, Yong-Wei Zhang, *Decoupled electron and phonon transports in hexagonal boron nitride-silicene bilayer heterostructure*. **J. Appl. Phys.** 119, 065102 (2016)
118. Nawat Suvansinpan, Fayyaz Hussain, Gang Zhang, Cheng Hsin Chiu, **Yongqing Cai*,** Yong-Wei Zhang*, *Substitutionally doped phosphorene: electronic properties and gas sensing*. **Nanotechnology** 27, 065708 (2016)
119. Guijian Guan, **Yongqing Cai**, Shuhua Liu, Haidong Yu, Shiqiang Bai, Yuan Cheng, Tao Tang, M. S. Bharathi, Yong-Wei Zhang, Ming-Yong Han, *High level incorporation of silver in gold nanoclusters: fluorescence red-shift upon interaction with hydrogen peroxide and fluorescence enhancement with herbicide*. **Chem. Eur. J.** 22, 1675–1681 (2016)
120. Yiling Yu, Yifei Yu, **Yongqing Cai**, Wei Li, Alper Gurarslan, Hartwin Peelaers, David E. Aspnes, Chris G. Van de Walle, Nhan V. Nguyen, Yong-Wei Zhang, and Linyou Cao, *Exciton-dominated dielectric function of atomically thin MoS_2 films*. **Sci. Rep.** 5, 16996 (2015)
121. Sandhya Chintalapati, **Yongqing Cai**, Ming Yang, Lei Shen, and Yuan Ping Feng, *Ferromagnetism of wide-bandgap semiconductor surfaces: Mg-doped AlN*. **Jpn. J. Appl. Phys**. 54, 110302 (2015)
122. Zhi Gen Yu, **Yongqing Cai**, and Yong-Wei Zhang, *Robust direct bandgap characteristics*

of one- and two-dimensional ReS_2. **Sci. Rep.** 5, 13783 (2015)

123. Chaoliang Tan, Peng Yu, Yanling Hu, Junze Chen, Ying Huang, **Yongqing Cai**, Zhimin Luo, Bing Li, Qipeng Lu, Lianhui Wang, Zheng Liu, and Hua Zhang, *High-yield exfoliation of ultrathin two-dimensional ternary chalcogenide nanosheets for highly sensitive and selective fluorescence DNA sensors*. **J. Am. Chem. Soc.** 137, 10430–10436 (2015)
124. Qingyun Wu, Lei Shen, Ming Yang, **Yongqing Cai**, Zhigao Huang, and Yuan Ping Feng, *Electronic and transport properties of phosphorene nanoribbons*. **Phys. Rev. B** 92, 035436 (2015)
125. Guijian Guan, Shuangyuan Zhang, Shuhua Liu, **Yongqing Cai**, Michelle Low, Choon Peng Teng, In Yee Phang, Yuan Cheng, Koh Leng Duei, Bharathi Madurai Srinivasan, Yuangang Zheng, Yong-Wei Zhang, and Ming-Yong Han, *Protein induces layer-by-layer exfoliation of transition metal dichalcogenides*. **J. Am. Chem. Soc.** 137, 6152-6155 (2015) **(Highly Cited Paper in Chemistry according to ISI)**
126. Wen Xu, Liyan Zhu, **Yongqing Cai**, Gang Zhang, and Baowen Li, *Direction dependent thermal conductivity of monolayer phosphorene: Parameterization of Stillinger-Weber potential and molecular dynamics study*. **J. Appl. Phys.** 117, 214308 (2015)
127. **Yongqing Cai**, Gang Zhang, and Yong-Wei Zhang, *Electronic properties of phosphorene/graphene and phosphorene/hexagonal boron nitride heterostructures*. **J. Phys. Chem.** C 119, 13929-13936 (2015)
128. **Yongqing Cai**, Qingqing Ke, Gang Zhang, Yuan Ping Feng, Vivek B. Shenoy, and Yong-Wei Zhang, *Giant phononic anisotropy and unusual anharmonicity of phosphorene: Interlayer coupling and strain engineering*. **Adv. Funct. Mater.** 25, 2230-2236 (2015) **(Selected as journal Cover) (Highly Cited Paper in Materials Science according to ISI)**
129. **Yongqing Cai**, Qingqing Ke, Gang Zhang, and Yong-Wei Zhang, *Energetics, charge transfer and magnetism of small molecules physisorbed on phosphorene*. **J. Phys. Chem. C** 119, 3102–3110 (2015) **(Highly Cited Paper in Chemistry according to ISI)**
130. Guijian Guan, Michelle Low, Shuhua Liu, **Yongqing Cai**, Shuangyuan Zhang, Dongsheng Geng, Cui Liu, Zhongping Zhang, Yuan Cheng, Madurai Srinivasan Bharathi, Yong-Wei Zhang, and Ming-Yong Han, *Destabilization of thiolated gold clusters for the growth of single-crystalline gold nanoparticles and their self-assembly for SERS detection*. **Part. Part. Syst. Charact.** 32, 588–595 (2015)
131. Qingqing Ke, Amit Kumar, Xiaojie Lou, Yuan Ping Feng, Kaiyang Zeng, **Yongqing Cai***, John Wang*, *Microstructural evolution of charged defects in the fatigue process of polycrystalline $BiFeO_3$ thin films.* **Acta Mater.** 82, 190–197 (2015)
132. Zhun-Yong Ong†, **Yongqing Cai**†, Gang Zhang, Yong-Wei Zhang, *Strong thermal transport anisotropy and strain modulation in single-layer phosphorene.* **J. Phys. Chem. C** 118, 25272−25277 (2014) **(Highly Cited Paper in Chemistry according to ISI)**
133. Zhaoqiang Bai, Lei Shen, **Yongqing Cai**, Qingyun Wu, Minggang Zeng, Guchang Han, Yuan Ping Feng, *Magnetocrystalline anisotropy and its electric-field assisted switching of Heusler-compound-based perpendicular magnetic tunnel junctions.* **New J. Phy.** 16103033 (2014)
134. Fayyaz Hussain, M. Imran, **Y. Q. Cai**, Hafeez Ullah, Abdul Shakoor, M. Rashid, Ejaz Ahmad, S. A. Ahmad, *Electronic properties of two-dimensional ZnO atomically sheet on Cu substrate: a first-principles study*. **Mod. Phys. Lett. B** 28, 1450204 (2014)
135. **Yongqing Cai**, Gang Zhang, Yong-Wei Zhang, *Layer-dependent band alignment and work function of few-layer phosphorene.* **Sci. Rep.** 4, 6677 (2014) **(Highly Cited Paper in Physics according to ISI)**
136. Zongyou Yin,† Xiao Zhang,† **Yongqing Cai**†, Junze Chen, Jen It Wong, Yee-Yan Tay, Jianwei Chai, Jumiati Wu, Zhiyuan Zeng, Bing Zheng, Hui Ying Yang, Hua Zhang,

Preparation of MoS_2–MoO_3 hybrid nanomaterials for light-emitting diodes. **Angew. Chem.** 53, 12560-12565 (2014)

137. Jinghua Lan, **Yongqing Cai**, Gang Zhang, Jian-Sheng Wang, Yong-Wei Zhang, *Topological symmetry-induced width dependence of the thermal conductance of edge-reconstructed graphene nanoribbons*. **J. Phys. D: Appl. Phys** 47, 265303 (2014)
138. Fayyaz Hussain, **Yongqing Cai**, M. Junaid Iqbal Khan, Muhammad Imran, Muhammad Rashid, Hafeez Ullah, Ejaz Ahmad, Farhana Kousard, S. A. Ahmad, *Enhanced ferromagnetic properties of Cu doped two-dimensional GaN monolayer*. **Int. J. Mod. Phys. C** 26, 1550009 (2014)
139. Guijian Guan, Shuang-Yuan Zhang, **Yongqing Cai**, Shuhua Liu, M. S. Bharathi, Michelle Low, Yong Yu, Jianping Xie, Yuangang Zheng, Yong-Wei Zhang, Ming-Yong Han, *Convenient purification of gold clusters by co-precipitation for improved sensing of hydrogen peroxide, mercury ions and pesticides*. **Chem. Commun.** 50, 5703-5705 (2014)
140. **Yongqing Cai**, Gang Zhang, Yong-Wei Zhang, *Polarity-reversed robust carrier mobility in monolayer MoS_2 nanoribbons*. **J. Am. Chem. Soc.** 136, 6269−6275 (2014) **(Highly Cited Paper in Chemistry according to ISI)**
141. Congwei Xie, Qingfeng Zeng, Dong Dong, Shuang Gao, **Yongqing Cai**, Artem R.Oganov, *First-principles calculations of the dielectric and vibrational properties of ferroelectric and paraelectric $BaAl_2O_4$*. **Phys. Lett. A** 378,1867–1870 (2014)
142. Guijian Guan, Shuhua Liu, **Yongqing Cai**, Michelle Low, M. S. Bharathi, Shuang-Yuan Zhang, Shiqiang Bai, Yong-Wei Zhang, Ming-Yong Han, *Destabilization of gold clusters for controlled nanosynthesis: From clusters to polyhedral*. **Adv. Mater.** 26, 3427–3432 (2014)
143. **Yongqing Cai**, Jinghua Lan, Gang Zhang, Yong-Wei Zhang, *Lattice vibrational modes and phonon thermal conductivity of monolayer MoS_2*. **Phys. Rev. B** 89, 035438 (2014) **(Highly Cited Paper in Physics according to ISI)**
144. **Yongqing Cai**, Zhaoqiang Bai, Hui Pan, Yuan Ping Feng, Boris I. Yakobson, Yong-Wei Zhang, *Constructing metallic nanoroad on MoS_2 monolayer via hydrogenation.* **Nanoscale** 6, 1691-1697 (2014) **(Highlighted in *Science Daily*, *A*STAR Research*)**
145. Zhaoqiang Bai, **Yongqing Cai**, Lei Shen, Guchang Han, Yuan Ping Feng, *High-performance giant-magnetoresistance junctions based on the all-Heusler architecture with matched energy bands and Fermi surfaces.* **Appl. Phys. Lett.** 102, 152403 (2013)
146. **Yongqing Cai**, Zhaoqiang Bai, Sandhya Chintalapati, Qingfeng Zeng, Yuan Ping Feng, *Transition metal atoms pathways on rutile TiO_2 (110) surface: Distribution of Ti^{3+} states and evidence of enhanced peripheral charge accumulation.* **J. Chem. Phys.** 138, 154711 (2013)
147. Muhammad Imran, Fayyaz Hussain, Muhammad Rashid, **Yongqing Cai**, S. A. Ahmad, *Mechanical behavior of Cu-Zr bulk metallic glasses (BMGs): A molecular dynamics approach*. **Chin. Phys. B** 22, 096101 (2013)
148. Bablu Mukherjee, **Yongqing Cai**, Hui Ru Tan, Yuan Ping Feng, Eng Soon Tok, Chorng Haur Sow, *NIR schottky photodetectors based on individual single-crystalline GeSe nanosheet*. **ACS Appl. Mater. Interfaces** 5, 9594−9604 (2013)
149. Bablu Mukherjee, Zhibin Hu, Minrui Zheng, **Yongqing Cai**, Yuan Ping Feng, Eng Soon Tok, Chorng Haur Sow, *Stepped-surfaced $GeSe_2$ nanobelts with high-gain photoconductivity*. **J. Mater. Chem.** 22, 24882-24888 (2012)
150. **Yongqing Cai**, Zhaoqiang Bai, Ming Yang, Yuan Ping Feng, *Effect of interfacial strain on spin injection and spin polarization of $Co_2CrAl/NaNbO_3/Co_2CrAl$ magnetic tunneling junction*. **EPL** 99, 37001 (2012)
151. Zhaoqiang Bai, **Yongqing Cai**, Lei Shen, M Yang, Viloane Ko, Guchang Han, and Yuan ping Feng, *Magnetic and transport properties of $Mn_{3-x}Ga/MgO/Mn_{3-x}Ga$ magnetic tunnel*

junctions: A first-principles study. **Appl. Phys. Lett.** 100, 022408 (2012)

152. Dechun Li, Ming Yang, Shengzhi Zhao, **Yongqing Cai**, Yunhao Lu, Zhaoqiang Bai, Yuanping Feng, *First-principles study of the effect of BiGa heteroantisites in GaAs:Bi alloy*. **Comput. Mater. Sci.** 63, 178–181 (2012)
153. Dechun Li, M. Yang, **Yongqing Cai,** Shengzhi Zhao, Yuanping Feng, *First principles study of the ternary complex model of EL2 defect in GaAs saturable absorber*. **Optics Express** 20, 6258 (2012)
154. Argo Nurbawono, Aihua Zhang, **Yongqing Cai**, Yihong Wu, Yuan Ping Feng, Chun Zhang, *Nanowelding of carbon nanotube-metal contacts: An effective way to control the Schottky barrier and performance of carbon nanotube based field effect transistors*. **J. Chem. Phys.** 136, 174704 (2012)
155. Dechun Li, Ming Yang, Shengzhi Zhao, **Yongqing Cai**, Yuanping Feng, *First principles study of Bismuth alloying effects in GaAs saturable absorber*. **Optics Express** 20, 11574 (2012)
156. Zhaoqiang Bai, **Yongqing Cai**, Lei Shen, Guchang Han, Yuanping Feng, An All-Heusler Design Scheme for High-Performance CPP-GMR Read Head, Digest Asia-Pacific Magnetic Recording Conference (APMRC), Singapore, from 2012-10-31 to 2012-11-02
157. Miao Zhou, **Yongqing Cai**, Minggang Zeng, Chun Zhang, Yuanping Feng, *Mn-doped thiolated Au-25 nanoclusters: Atomic configuration, magnetic properties, and a possible high-performance spin filter*. **Appl. Phys. Lett.** 98, 143103 (2011)
158. Miao Zhou, Yun-Hao Lu, **Yong-Qing Cai**, Chun Zhang, Yuan-Ping Feng, *Adsorption of gas molecules on transition metal embedded graphene: a search for high-performance graphene-based catalysts and gas sensors.* **Nanotechnology** 22, 385502 (2011)
159. **Yongqing Cai**, Aihua Zhang, Yuan Ping Feng, Chun Zhang, *Switching and rectification of a single light-sensitive diarylethene molecule sandwiched between graphene nanoribbons.* **J. Chem. Phys**. 135, 184703 (2011)
160. **Yongqing Cai**, Miao Zhou, Minggang Zeng, Chun Zhang, Yuan Ping Feng, *Adsorbate and defect effects on electronic and transport properties of gold nanotubes.* **Nanotechnology** 22, 215702 (2011)
161. Qingfeng Zeng, Litong Zhang, Xian Zhang, Qichao Chen, Zhiqiang Feng, **Yongqing Cai,** Laifei Cheng, Zuohai Weng, *Vibrational and dielectric properties of magnesium aluminate spinel: A first-principles study*. **Phys. Lett. A** 375, 3521-3524 (2011)
162. **Yongqing Cai**, Chun Zhang, Yuan Ping Feng, *Dielectric properties and lattice dynamics of α-PbO_2-type TiO_2: The role of soft phonon modes in pressure-induced phase transition to baddeleyite-type TiO_2.* **Phys. Rev. B** 84, 094107 (2011)
163. Minggang Zeng, Lei Shen, **Yongqing Cai**, Zhendong Sha, Yuanping Feng, *Perfect spin filter and spin-valve in carbon atomic chains.* **Appl. Phys. Lett.** 96, 042104 (2010)
164. **Yongqing Cai**, Aihua Zhang, Yuan Ping Feng, Chun Zhang, Hao Fatt Teoh, GhimWei Ho, *Strain effects on work functions of pristine and potassium-decorated carbon nanotubes.* **J. Chem. Phys.** 131, 224701 (2009) **(Selected as journal Cover)**
165. Yunhao Lu, Rongqin Wu, Lei Shen, Ming Yang, Zhendong Sha, **Yongqing Cai**, Pimo He, Yuanping Feng, *Effects of edge passivation by hydrogen on electronic structure of armchair graphene nanoribbon and band gap engineering.* **Appl. Phys. Lett.** 94, 122111 (2009)
166. Zhendong Sha, Rongqin Wu, Yunhao Lu, Lei Shen, Ming Yang, **Yongqing Cai**, Yuanping Feng, Yi Li, *Glass forming abilities of binary $Cu_{100-x}Zr_x$ (34, 35.5, and 38.2 at. %) metallic glasses: A LAMMPS study*. **J. Appl. Phys**. 105, 043521 (2009)
167. Ming Yang, Rongqin Wu, Wensheng Deng, Lei Shen, Zhendong Sha, **Yongqing Cai**, Yuanping Feng, Shijie Wang, *Electronic structures of ß-Si_3N_4(0001)/Si(111) interfaces: Perfect bonding and dangling bond effects.* **J. Appl. Phys.** 105, 024108 (2009)

168. R. Q. Wu, L. Shen, M. Yang, Z. D. Sha, **Y. Q. Cai**, Y. P. Feng, Z. G. Huang, Q. Y. Wu, *Enhancing hole concentration in AlN by Mg : O codoping: Ab initio study*. **Phys. Rev. B** 77, 073203 (2008)
169. R. Q. Wu, L. Shen, M. Yang, Z. D. Sha, **Y. Q. Cai,** Y. P. Feng, Z. G. Huang, Q. Y. Wu, *Possible efficient p-type doping of AlN using Be: An ab initio study*. **Appl. Phys. Lett.** 91, 152110 (2007)
170. **Yongqing Cai**, Litong Zhang, Qingfeng Zeng, Laifei Cheng, Yongdong Xu, *Infrared reflectance spectrum of BN calculated from first principles*. **Solid State Commun.** 141, 262 (2007)
171. **Yongqing Cai,** Litong Zhang, Qingfeng Zeng, Laifei Cheng, Yongdong Xu, *First-principles study of vibrational and dielectric properties of ß-Si_3N_4*. **Phys. Rev. B** 74, 174301 (2006)

CONFERENCES /WORKSHOP /TALKS

1. **(Keynote) Yongqing Cai**, "Atomic Mechanisms of the Modulation of Properties of Low-dimensional Materials from First-principles Simulations", International Forum on Condensed Matter Physics, Webinar, 06 February 2023
2. **(Keynote) Yongqing Cai**, "Exploration of the Two-Dimensional Materials from First-Principles", **Xiangjiang Academic Forum,** Hunan University of Science and Technology, Webinar, 04 December 2022
3. **(Keynote) Yongqing Cai**, "Modulation of the Electronic Properties of TwoDimensional Materials Via Strain and Chemical Functionalization", **2022 International Conference on Intelligent Material Design (ICIMD2022),** Webinar, 24-26 June 2022
4. **(Invited) Yongqing Cai**, "Impact of Surface/Interface of the Semiconducting Materials by First-principles Study",**第二屆中國光電信息功能材料與器件學術高峰論壇**，Qingdao University, Qingdao, Shandong Province, China, 31 July 2021-02 August 2021
5. Zhi Gen Yu, **Yongqing Cai**, Junfeng Gao, Lin Wang, Li Chen, Shuai Chen, Gang Zhang, Kah Wee Ang, Yong-Wei Zhang,"2D Semiconducting Materials for Nanoelectronics and Energy Applications", Vebleo Webinar, 23 January, 2021
6. (**Session co-chair, invited**) **Yongqing Cai**, "材料的界面以及缺陷的量子第一性原理研究"，**粵港澳高校聯盟 2020 年青年學者論壇-交叉科學理論與計算專業聯盟分論壇**，Sun Yat-Sen University/Online，27-28 November, 2020.
7. **(Invited) Yongqing Cai**, "Artificial Intelligence and Data-driven Materials Exploration", ***The 4th Forum of Materials Genome Engineering (ForMGE)***, Mianyang, Sichuan, China, 21-23 October, 2020.
8. **(Invited) Yongqing Cai**, "Exploring Defects and Interfaces of 2D Materials via Quantum Simulation", 科研新勢力線上講座論壇，http://live.bilibili.com/22237308, Webinar, 4 July, 2020.
9. **(Invited) Yongqing Cai**, "Quantum simulation of charge transfer and atomic motion in two-dimensional layered materials". ***2018 International Symposium on Science Research Aiming to Application of Ceramic Matrix Composite***. Xi'an, China, 14-17 April, 2018.
10. **Yongqing Cai**, Gang Zhang, Yong-Wei Zhang, "Phonons in phosphorene and InSe". ***The 9th International Conference on Materials for Advanced Technologies (ICMAT)***, Singapore, 16-20 January, 2017.
11. **(Invited)** Yong-Wei Zhang, **Yongqing Cai**, Junfeng Gao, Gang Zhang, Andrey A Kistanov, Kun Zhou, "Structure, defect, and growth of phosphorene: A first-principles exploration". ***The 9th International Conference on Materials for Advanced Technologies (ICMAT)***, Singapore, 16-20 January, 2017.
12. **(Invited)** Yong-Wei Zhang, **Yongqing Cai**, Junfeng Gao, Gang Zhang, Andrey A Kistanov, Kun Zhou, "Structure, defect, and growth of phosphorene: A first-principles exploration".

International Graphene Innovation Conference, Nanjing, China, 24-26 September 2017.

13. **(Invited)** **Yongqing Cai**, "Electronic and vibrational properties of MoS2 and phosphorene". ***The 10th International Conference on Computational Physics (ICCP10)***, Macau, China, 7-11 January 2017.
14. Andrey A. Kistanov, **Yongqing Cai**, Kun Zhou, Sergey V. Dmitriev, Narasimalu Srikanth, Danial Saadatmand, Yong-Wei Zhang, "Strain and defects engineering of phosphorene". ***2017 Asian Conference on Energy, Power and Transportation Electrification (ACEPT)***, Singapore, 24-26 Oct. 2017.
15. Gang Zhang, Xiangjun Liu, Zhun-Yong Ong, **Yongqing Cai**, Yong-Wei Zhang, "Thermal properties of 2D semiconductors—theory and application". ***Materials Research Society Spring Meeting***, Phoenix Arizona, USA, 17-21 April, 2017.
16. **Yongqing Cai**, "Phononic and electronic properties of phosphorene, A first-principles study". ***The 8th International Conference on Materials for Advanced Technologies (ICMAT)***, Singapore, 28 June - 3 July 2015.
17. **(Invited)** Yong-Wei Zhang, **Yongqing Cai**, Weifeng Li, Zhun-Yong Ong and Gang Zhang, "Strain-engineering two-dimensional semiconducting materials for nanoelectronics and energy conversion". ***Materials Research Society Spring Meeting***, San Francisco, USA, 6-10 April, 2015.
18. Zhaoqiang Bai, **Yongqing Cai**, Lei Shen, Guchang Han, Yuanping Feng, "An all-Heusler design scheme for high-performance CPP-GMR read heads", ***Asia-Pacific Magnetic Recording Conference (APMRC)***, Singapore, 31 Oct-2 Nov 2012.
19. Zhaoqiang Bai, **Yongqing Cai**, Viloane Ko, Guchang Han, and Yuanping Feng, "Magnetic and transport properties of Mn3-xGa/MgO/Mn3-xGa magnetic tunneling junctions: A first-principles study". ***The 6th Conference of the Asian Consortium on Computational Materials Science (ACCMS-6)***, Singapore, 6-9 September 2011.