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, 2023);
THEORY AND MODELING OF MATERIALS PROPERTIES (APAC4009), Undergraduate, University of Macau, Spring Semester (2023, 2024).

HONORS & AWARDS

2023 Stanford's top 2% most highly cited scientists 2023
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:

- Molecular dynamics and metadynamics
- 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
- Machine learning potential
- Advanced materials for energy applications

GRANTS COMPLETED

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. 2022,2023, 國家自然基金委評審專家
2. 07/03/2023, Pedagogic Activity, Scientific Talk at Escola Choi Nong Chi Tai (澳門菜農子弟學校)
3. 22/03/2023, English Table at Cheong Kun Lun College
4. 01/01/2023-now, Associate Editor, Computer Modeling in Engineering & Science (CMES)
5. 20/12/2022, Expert Committee Members, Global Youth Technology and Innovation Forum
6. 16/12/2022, Pedagogic Activity, Scientific Talk at Sacred Heart Canossian College (澳門嘉諾撒聖心女子中學)
7. 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委員
8. 14/10/2021-now, Editorial Board Members, Data
9. 31/03/2021, Guest Editor, Special Issue for 60th Anniversary Celebration, “Modelling of Low-dimensional Functional Nanomaterials”, *Physica Status Solidi (RRL) - Rapid Research Letters*
10. 12/03/2021, Pedagogic Activity, Scientific Talk at Yuet Wah College (澳門粵華中學) for whole college student
11. 02/2021-now, European Materials Modelling Council (EMMC), Associated Member
12. 16/12/2020, Pedagogic Activity, Tutorial at Cheong Kun Lun College
13. 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 Nanotechnology, 1 Nature Electronics, 2 Proceedings of the National Academy of Sciences, 1 Joule, 4 Nature Communications, 5 Journal of the American Chemical Society, 2 Angewandte Chemie, 3 ACS Nano, 1 Advanced Science, 5 Advanced Materials, 7 Advanced Functional Materials, 12 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	9500	12000
h-index	50	55
i10-index	97	129

*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. Zian Xu, Jian Zhu, Zheng Shu, Yu Xia, Rouxi Chen*, Shaoqing Chen, Yu Wang, Lin Zeng, Jiacheng Wang, **Yongqing Cai***, Shi Chen*, Fuqiang Huang*, and Hsing-Lin Wang*, *Phosphorus-induced anti-growth of ruthenium clusters-single atoms for ultra-stable hydrogen evolution over 100,000 cycles*. **Joule** 8, 1-14 (2024)
2. Huifang Xu, Qingbin Jiang, Zheng Shu, Kwan San Hui*, Shuo Wang, Yunshan Zheng,Xiaolu Liu, Huixian Xie, Weng-Fai Ip, Chenyang Zha, **Yongqing Cai***, and Kwun Nam Hui*, *Fundamentally manipulating the electronic structure of polar bifunctional catalysts for lithium-sulfur batteries: Heterojunction design versus doping engineering*. **Adv. Sci.** 2307995 (2024)
3. Xiangyue Cui, Hejin Yan, Xuefei Yan, Kun Zhou, **Yongqing Cai***, *Promoted electronic coupling of acoustic phonon modes in doped semimetallic $MoTe_2$*. **ACS Nano** 17, 16530–16538 (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. 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 Commun.** 14, 411 (2023)
6. 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)
7. 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.** 33, 2208528 (2022)
8. 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)
9. 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)

10. **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)
11. **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)**
12. **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. Zian Xu, Jian Zhu, Zheng Shu, Yu Xia, Rouxi Chen*, Shaoqing Chen, Yu Wang, Lin Zeng, Jiacheng Wang, **Yongqing Cai***, Shi Chen*, Fuqiang Huang*, and Hsing-Lin Wang*, *Phosphorus-induced anti-growth of ruthenium clusters-single atoms for ultra-stable hydrogen evolution over 100,000 cycles*. **Joule** 8, 1-14 (2024)
2. Haiyang Zhu, Hongfei Chen, Jianjian Fei, Yutong Deng, Tian Yang, Pinhao Chen, Ying Liang, **Yongqing Cai***, Lu Zhu*, and Zhanfeng Huang*, *Solution-processed CsPbBr3 perovskite films via CsBr intercalated $PbBr_2$ intermediate for high-performance photodetectors towards underwater wireless optical communication*. **Nano Energy** 125, 109513 (2024)
3. Huifang Xu, Qingbin Jiang, Zheng Shu, Kwan San Hui*, Shuo Wang, Yunshan Zheng, Xiaolu Liu, Huixian Xie, Weng-Fai Ip, Chenyang Zha, **Yongqing Cai***, and Kwun Nam Hui*, *Fundamentally manipulating the electronic structure of polar bifunctional catalysts for lithium-sulfur batteries: Heterojunction design versus doping engineering*. **Adv. Sci.** 2307995 (2024)
4. Zheng Shu, Huaxian Jia, Zhongheng Li, Bowen Wang, and **Yongqing Cai***, *Exotic quartic anharmonicity induced by rattling effect in layered isostructural compounds*. **J. Phys. Chem. C** 128, 11, 4809–4817 (2024)
5. Jie Huang, Bowen Wang, Hejin Yan, and **Yongqing Cai***, *Mechanism of interaction of water above methylammonium lead iodide perovskite nanocluster: Size effect and water-induced defective states*. **J. Phys. Chem. Lett**. 15, 575–582 (2024)
6. Changmeng Huan, Zihan Lu, Silin Tang, **Yongqing Cai***, and Qingqing Ke*, *Facile intercalation of alkali ions in WO_3 for modulated electronic and optical properties: Implications for artificial synapses and chromogenic application*. **Sci. China Phys. Mech. Astron.** 67, 227311 (2024)
7. Silin Tang, Yingzhi Meng, **Yongqing Cai**, Biaolin Peng, Laijun Liu, and Qingqing Ke, *Achieving improved electrocaloric effect and broad operation temperature by tailoring phase fraction in $BaTiO_3$-based ceramics*. **Ceram. Int.** 50, 10825-10834 (2024)
8. Zheng Shu, Huifang Xu, Hejin Yan, and **Yongqing Cai***, *Strong anisotropy of thermal transport in the monolayer of a new puckered phase of PdSe*. **Front. Phys.** 19, 33202 (2024)
9. Qiye Guan and **Yongqing Cai***, *Nanopore rigidity as an atomic descriptor of ion-transfer kinetics in sieving membranes: Insights from two-dimensional g-C_3N_4*. **Mater. Today Nano** 25, 100437 (2024)
10. Hanyan Fang, Harshitra Mahalingam, Xinzhe Li, Xu Han, Zhizhan Qiu, Yixuan Han, Keian Noori, Dikshant Dulal, Hongfei Chen, Pin Lyu, Tianhao Yang, Jing Li, Chenliang Su, Wei Chen, **Yongqing Cai**, Antonio Castro H. Neto, Kostya S. Novoselov, Aleksandr Rodin, and

Jiong Lu, *Atomically-precise vacancy-assembled quantum antidots*. **Nature Nanotech.** 18, 1401-1408 (2023)

11. Yulan Huang, Bingzhe Wang, Tanghao Liu, Dongyang Li, Yujie Zhang, Tianqi Zhang, Xiyu Yao, Yun Wang, Abbas Amini, **Yongqing Cai**, Baomin Xu, Zikang Tang, Guichuan Xing, and Chun Cheng, *Stabilization of α-phase $FAPbI_3$ via buffering interfacial region for efficient p–i–n perovskite solar cells.* **Adv. Funct. Mater**. 33, 2302375 (2023)
12. Xiangyue Cui, Hejin Yan, Xuefei Yan, Kun Zhou, and **Yongqing Cai***, *Promoted electronic coupling of acoustic phonon modes in doped semimetallic $MoTe_2$*. **ACS Nano** 17, 16530–16538 (2023)
13. Xiangyue Cui, and **Yongqing Cai***, *Computational study of strong phonon softening and electron–phonon interaction in doped monolayer tellurene: Implications for neuromorphic applications.* **ACS Appl. Nano Mater.** 6, 17457–17463 (2023)
14. Hongfei Chen, Hejin Yan, and **Yongqing Cai***, *Recipe for the design of mixed cation lead halide perovskites: adsorption and charge transfer from A-site cations to PbI_2.* **J. Mater. Chem. A** 11, 19349 - 19359 (2023)
15. Hongfei Chen, Qiye Guan, Hejin Yan, Xiangyue Cui, Zheng Shu, and **Yongqing Cai***, *Additive molecules adsorbed on monolayer PbI_2: atomic mechanism of solvent engineering for perovskite solar cells.* **ACS Appl. Mater. Interfaces** 15, 32475–32486 (2023)
16. 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)
17. Xuefei Yan, Xiangyue Cui, Bowen Wang, Hejin Yan, **Yongqing Cai***, and Qingqing Ke*, *Surface asymmetry induced turn-overed lifetime of acoustic phonons in monolayer MoSSe*. **iScience**, 26, 106731 (2023)
18. Bingtao Liu, Hanxi Sun, Changmeng Huan, Renxu Jia, **Yongqing Cai**, and 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)
19. Zheng Shu, Hongfei Chen, Xing Liu, Huaxian Jia, Hejin Yan, and **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)
20. 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)
21. 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)
22. 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)
23. 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)
24. 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)

25. 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)
26. Ruxin Guo, Junmin Xia, Hao Gu, Xuke Chu, Yan Zhao, Xianghuan Meng, Zhiheng Wu, Jiangning Li, Yanyan Duan, Zhenzhen Li, Zhaorui Wen, Shi Chen, and **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)
27. 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)
28. Zheng Shu, Bowen Wang, Xiangyue Cui, Xuefei Yan, Hejin Yan, Huaxian Jia, and **Yongqing Cai***, *High-performance thermoelectric monolayer γ-GeSe and its group-IV monochalcogenide isostructural family.* **Chem. Eng. J.** 454, 140242 (2023)
29. 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)
30. Kangdi Niu, Guotao Qiu, Chuanshou Wang, Daiyue Li, Yutao Niu, Songge Li, Lixing Kang, **Yongqing Cai***, Mengjiao Han*, and Junhao Lin*, *Self-intercalated magnetic heterostructures in 2D chromium telluride*. **Adv. Funct. Mater.** 33, 2208528 (2022)
31. Ziqing Ye, Junmin Xia, Dengliang Zhang, Xingxing Duan, Zhaohui Xing, Guangrong Jin, **Yongqing Cai**, Guichuan Xing, Jiangshan Chen, and Dongge Ma, *Efficient quasi-2D perovskite light-emitting diodes enabled by regulating phase distribution with a fluorinated organic cation*. **Nanomaterials** 12, 3495 (2022)
32. 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)
33. 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)
34. 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)
35. 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)
36. 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)
37. 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)
38. 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)
39. 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)
40. 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)

41. 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).
42. Xiaozong Hu, Kailang Liu, **Yongqing Cai**, Shuang-Quan Zang, Tianyou Zhai, *2D Oxides for Electronics and Optoelectronics*. **Small Science** 2, 2200008 (2022)
43. 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)
44. 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)
45. 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)
46. 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)
47. 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)
48. 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)
49. 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)
50. 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)
51. 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)
52. 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)
53. 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)
54. 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)
55. 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)

56. Kun Zhou*, Bo Liu*, **Yongqing Cai***, Sergey V. Dmitriev*, Shaofan Li*, *Modelling of low-dimensional functional nanomaterials*. **Phys. Status Solidi RRL** 16, 2100654 (2022)
57. 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)
58. 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)
59. 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)
60. 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)
61. 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)
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CONFERENCES /WORKSHOP /TALKS

1. **(Invited) Yongqing Cai,** "First-Principles Study on Structural and Electronic Properties in Layered Materials", ***International Collaborative Seminar on Future Materials and Forming Technologies Development***, Wuhan, China, 3-4 December 2023
2. **(Invited) Yongqing Cai,** 騰沖科學家論壇, 雲南騰沖, 30 November-02 December 2023
3. Guotao Qiu, Hejin Yan, Zheng Shu, Bowen Wang, **(Invited) Yongqing Cai,** "Ferroic Order in Two-dimensional Materials: Perspective from First-principles Study", ***The 13th Asian Meeting on Ferroelectrics jointly with the 13th Asian Meeting on Electroceramics (AMF-13 & AMEC-13)***, Macau, 12-16 November 2023
4. **(Invited) Yongqing Cai,** 新時代理論與計算化學的挑戰和機遇研討會, Hanzhong, China, 3-7 August 2023
5. **Yongqing Cai,** Jiaren Yuan, Hejin Yan, Yuan Ping Feng, "Bond Distortion and Reconstruction in Two dimensional Materials Perspective from First principles Study", ***The 11th International Conference on Materials for Advanced Technologies (ICMAT)***, Singapore, 26-30 June 2023.

6. **(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
7. **(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
8. **(Keynote) Yongqing Cai**, "Modulation of the Electronic Properties of TwoDimensional Materials Via Strain and Chemical Functionalization", ***International Conference on Intelligent Material Design (ICIMD2022),*** Webinar, 24-26 June 2022
9. **(Invited) Yongqing Cai**, "Impact of Surface/Interface of the Semiconducting Materials by First-principles Study",**第二届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
10. 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
11. (**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.
12. **(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.
13. **(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.
14. **(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.
15. **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.
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19. 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.
20. 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.
21. **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.

22. **(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.
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24. 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.