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Education

09/1999 to 10/2003	Ph.D., The University of Hong Kong, Hong Kong
09/1996 to 05/1999	B.Sc. in Chemistry with first class honor, The University of Hong Kong, Hong Kong

Work Experience

09/2019 to now	**Associate Professor, Beijing Computational Science Research Center**, Beijing
03/2013 to 08/2019	**Assistant Professor, Beijing Computational Science Research Center**, Beijing
04/2010 to 03/2013	**Research Assistant Professor, The University of Hong Kong**, Hong Kong
04/2009 to 03/2010	**Post-doctoral Fellow, University of Bremen**, Bremen
02/2004 to 03/2009	**Post-doctoral Fellow, The University of Hong Kong**, Hong Kong

Awards

2014	NSFC Excellent Young Researcher Award
2013	1000 Young Talent Program of China

Research Grants

2020 to 2022	Guangdong-Shenzhen Joint Key Project Funding (Grant no. 2019B1515120045)
	Title: Multiscale Modeling of Optoelectronic Devices
	Role: PI
2017 to 2020	NSFC General Program (Grant no. 21673017)
	Title: Coupled Optical-Electrical Study of Plasmonic Nanoscale Solar Cells
	Role: PI
2014-2016	NSFC Excellent Young Researcher (Grant no. 21322306)
	Title: Multiscale Simulation of Complex Systems
	Role: PI
2014-2019	National Basic Research Program of China (Grant no. 2014CB921402)
	Title: Basic Device Physics of Solid-State Quantum Computing
	Role: Co-I

Publications

1. Xiaoyan Wu, Rulin Wang, Na Liu, Hao Zou, Bin Shao, Lei Shao and **ChiYung Yam**
   Controlling the emission frequency of graphene nanoribbon emitters based on spatially excited topological boundary states
   Phys. Chem. Chem. Phys. 2020, 22, 8277-8283 (Front Cover)

2. Hai Bi, Carlos-Andres Palma, Yuxiang Gong, Klara Stallhofer, Matthias Nuber, Chao Jing, Felix Meggendorfer, Shizheng Wen, **ChiYung Yam**, Reinhard Kienberger, Mark Elbing, Marcel Mayor, Hristo Iglev, Johannes V Barth and Joachim Reichert
   Electron-phonon coupling in current-driven single-molecule junctions
   J. Am. Chem. Soc. 2020, 142, 3384-3391

3. Zhao Liu, **ChiYung Yam**, Shiwu Gao, Tao Sun and Dong-Bo Zhang
   Lattice dynamics of twisted ZnO nanowires under generalized Born–von Karman boundary conditions
   New J. Phys. 2020, 22 023004

4. Fuzhen Bi, **ChiYung Yam**, Chengjie Zhao, Le Liu, Min Zhao, Xiao Zheng and Tonggang Jiu
   Enhanced photocurrent in heterostructures formed between $CH_3NH_3PbI_3$ perovskite films and graphdiyne
   Phys. Chem. Chem. Phys. 2020, 22, 6239-6246

5. Shizheng Wen, Shiwu Gao and **ChiYung Yam**
   Serial and parallel spin circuits at the molecular scale with two atomic-vacancies in graphene: Amplification of spin-filtering effect
   Carbon 2020, 154, 357-362

6. Rulin Wang, Fuzhen Bi, Wencai Lu and **ChiYung Yam**
   Tunable photoresponse by gate modulation in bilayer graphene nanoribbon devices
   J. Phys. Chem. Lett. 2019, 10, 7719-7724

7. Ziyao Xu, Yi Zhou, Lynn Groß, Antonietta De Sio, **ChiYung Yam**, Christoph Lienau, Thomas Frauenheim and GuanHua Chen
   Coherent real-space charge transport across a donor-acceptor interface mediated by vibronic couplings
   Nano Lett. 2019, 19, 8630-8637

8. Bing Song, Limin Liu and **ChiYung Yam**
   Suppressed carrier recombination in Janus MoSSe bilayer stacks: a time-domain ab initio study
   J. Phys. Chem. Lett. 2019 10, 5564-5570

9. Xiaoyan Wu, Rulin Wang, Yu Zhang, Bowen Song and **ChiYung Yam**
   Controllable single-molecule light emission by selective charge injection in scanning tunneling microscopy
   J. Phys. Chem. C 2019, 123, 15761-15768

10. Sateesh Bandaru, Ivan Scivetti, **ChiYung Yam** and Gilberto Teobaldi
    The role of isotropic and anisotropic Hubbard corrections for the magnetic ordering and absolute band alignment of hematite α-Fe_2O_3 (0001) surfaces
    Prog. Nat. Sci-Mater. 2019, 29, 349-355

11. Rulin Wang, Wencai Lu, Hang Xie, Xiao Zheng and **ChiYung Yam**
    Theoretical investigation of real-time charge dynamics in open systems coupled to bulk materials
    J. Chem. Phys. 2019, 150, 174119

12. Fuzhen Bi, Xiao Zheng and **ChiYung Yam**
    First-principles study of mixed cation methylammonium-formamidinium hybrid perovskite
    Acta Phys-Chim Sin. 2019, 35, 69-75

13. Govindarajan Saranya, **ChiYung Yam**, Shiwu Gao and Mingyang Chen
    Roles of chenodeoxycholic acid coadsorbent in anthracene-based dye-sensitized solar cells: a density functional theory study
    J. Phys. Chem. C 2018, 122, 23280-23287

14. Sateesh Bandaru, Govindarajan Saranya, Niall J. English, **ChiYung Yam** and Mingyang Chen
    Tweaking the electronic and optical properties of α-MoO_3 by sulphur and selenium doping–a density functional theory study
    Sci. Rep. 2018, 8, 1-12

15. Shizheng Wen, Fei Gao, **ChiYung Yam** and Shiwu Gao
    Nanomechanical control of spin current flip using monovacancy graphene
    Carbon 2018, 133, 218-223

16. Jia En Lu, Chou-Hsun Yang, Haobin Wang, **ChiYung Yam**, Zhi-Gang Yu and Shaowei Chen
    Plasmonic circular dichroism of vesicle-like nanostructures by the template-less self-assembly of achiral Janus nanoparticles
    Nanoscale 2018, 10, 14586-14593

17. Na Liu and **ChiYung Yam**
    First-principles study of intrinsic defects in formamidinium lead triiodide perovskite solar cell absorbers
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18. Chou-Hsun Yang, **ChiYung Yam** and Haobin Wang
    Approximate DFT-based methods for generating diabatic states and calculating electronic couplings: models of two and more states
    Phys. Chem. Chem. Phys. 2018, 20, 2571-2584

19. Fuzhen Bi, Stanislav Markov, Rulin Wang, YanHo Kwok, Weijun Zhou, Limin Liu, Xiao Zheng, GuanHua Chen and **ChiYung Yam**
    Enhanced photovoltaic properties induced by ferroelectric domain structures in organometallic halide perovskites
    J. Phys. Chem. C 2017 121, 11151-11158

20. Lingyi Meng, Yu Zhang and **ChiYung Yam**
Multiscale study of plasmonic scattering and light trapping effect in silicon nanowire array solar cells
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21. Saranya Govindarajan, Shiwu Gao, Wei Cai and **ChiYung Yam**
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22. Rulin Wang, Yu Zhang, Fuzhen Bi, Thomas Frauenheim, GuanHua Chen and **ChiYung Yam**
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23. Yu Zhang, **ChiYung Yam** and George C. Schatz
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24. Bang-Ming Ming, Ru-Zhi Wang, **ChiYung Yam**, Li-Chun Xu, Woon-Ming Lau and Hui Yan
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25. Jianping Xiao, Liangzhi Kou, **ChiYung Yam**, Thomas Frauenheim and Binghai Yan
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27. Rulin Wang, Xiao Zheng, YanHo Kwok, Hang Xie, GuanHua Chen and **ChiYung Yam**
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48. Lingyi Meng, **ChiYung Yam**, SiuKong Koo, Quan Chen, Ngai Wong and GuanHua Chen
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Time-dependent density-functional theory for open systems
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