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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

2021 to 2024	NSFC General Program (Grant no. 22073007) Title: Time-domain method development and its application for nanoscale optoelectronic devices Amount: 630K RMB Role: PI 2021 - 2024
2020 to 2022	Guangdong-Shenzhen Joint Key Project Funding (Grant no. 2019B1515120045) Title: Multiscale Modeling of Optoelectronic Devices Amount: 1M RMB Role: PI 2020 - 2022
2017 to 2020	NSFC General Program (Grant no. 21673017) Title: Coupled Optical-Electrical Study of Plasmonic Nanoscale Solar Cells Amount: 650K RMB Role: PI 2017 - 2020
2014 to 2016	NSFC Excellent Young Researcher (Grant no. 21322306) Title: Multiscale Simulation of Complex Systems Amount: 1M RMB Role: PI 2014 - 2016
2014 to 2019	National Basic Research Program of China (Grant no. 2014CB921402) Title: Basic Device Physics of Solid-State Quantum Computing Amount: 1.23M RMB Role: Co-I 2014 - 2019

Teaching Experience

2020 – 2021	**The University of Hong Kong** Physical Chemistry: Introduction to Quantum Chemistry
2016 – 2019	**Beijing Computational Science Research Center** Graduate Course: Parallel Algorithms for Scientific Computing
Nov 2014	**Hong Kong University of Science and Technology** Guest Lectures: Quantum Chemistry
2010 – 2012	**The University of Hong Kong** Physical Chemistry I: Chemical Kinetics, Chemical Equilibrium

Five Representative Publications

1. Rulin Wang, Fuzhen Bi, Wencai Lu, Xiao Zheng and **ChiYung Yam**
   Tracking electron dynamics of single molecules in scanning tunneling microscopy junctions with laser pulses
   J. Phys. Chem. Lett. 2021, 12, 6398-6404

2. Yuxiang Liu, Jin Zhang, Sheng Meng, **ChiYung Yam** and Thomas Frauenheim
   Electric field tunable ultrafast interlayer charge transfer in graphene/WS_2 heterostructure
   Nano Lett. 2021, 21 4403-4409

3. 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)

4. 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

5. Lingyi Meng, Yu Zhang and **ChiYung Yam**
   Multiscale study of plasmonic scattering and light trapping effect in silicon nanowire array solar cells
   J. Phys. Chem. Lett. 2017, 8, 571-575

Full Publication List

1. Rulin Wang, Fuzhen Bi, Wencai Lu, Xiao Zheng and **ChiYung Yam**
   Tracking electron dynamics of single molecules in scanning tunneling microscopy junctions with laser pulses
   J. Phys. Chem. Lett. 2021, 12, 6398-6404

2. Yuxiang Liu, Jin Zhang, Sheng Meng, **ChiYung Yam** and Thomas Frauenheim
   Electric field tunable ultrafast interlayer charge transfer in graphene/WS_2 heterostructure
   Nano Lett. 2021, 21 4403-4409

3. Ziyao Xu, Yi Zhou, **ChiYung Yam**, Lynn Gross, Antonietta De Sio, Thomas Frauenheim, Christoph Lienau and Guanhua Chen
   Revealing generation, migration, and dissociation of electron-hole pairs and current emergence in an organic photovoltaic cell
   Sci. Adv. 2021, 7, eabf7672

4. Baishun Yang, Bin Shao, Jianfeng Wang, Yang Li, **ChiYung Yam**, Shengbai Zhang and Bing Huang
   Realization of semiconducting layered multiferroic heterojunctions via asymmetrical magnetoelectric coupling
   Phys. Rev. B 2021, 103, L201405

5. Sa Zhang, Jianfeng Wang, Shizheng Wen, Ming Jiang, Haiyan Xiao, Xiang Ding, Ning Wang, Menglu Li, Xiaotao Zu, Sean Li, **ChiYung Yam**, Bing Huang and Liang Qiao
   Approaching charge separation efficiency to unity without charge recombination
   Phys. Rev. Lett. 2021, 126, 176401

6. Xuelei Sui, Jianfeng Wang, **ChiYung Yam** and Bing Huang
   Two-dimensional magnetic anionic electrons in electrides: generation and manipulation
   Nano Lett. 2021, 21, 3813-3819

7. Jia-Jia Yang, Xiang-Yang Liu, Zi-Wen Li, Thomas Frauenheim, **ChiYung Yam**, Wei-Hai Fang and Ganglong Cui
   The spin-orbit interaction controls photoinduced interfacial electron transfer in fullerene-perovskite heterojunctions: C_{60} versus C_{70}
   Phys. Chem. Chem. Phys. 2021, 23, 6536-6543

8. Lingyi Meng and **ChiYung Yam**
   Multiscale Quantum Mechanics/Electromagnetics Method for the Simulation of Photovoltaic Devices
   Computational Materials, Chemistry, and Biochemistry: From Bold Initiatives to the Last Mile, page 693-715 (Springer, 2021)

9. Lei Cui, Rulin Wang, **ChiYung Yam**, GuanHua Chen and Xiao Zheng
   Quantum Mechanical Simulation of Electron Dynamics on Surfaces of Materials
   Computational Materials, Chemistry, and Biochemistry: From Bold Initiatives to the Last Mile, page115-136 (Springer, 2021)

10. 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)

11. 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

12. 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

13. 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

14. 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

15. 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

16. 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

17. 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

18. 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

19. 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

20. 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

21. 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

22. 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

23. 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

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

25. 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

26. Na Liu and **ChiYung Yam**
First-principles study of intrinsic defects in formamidinium lead triiodide perovskite solar cell absorbers
Phys. Chem. Chem. Phys. 2018, 20, 6800-6804

27. 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

28. 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

29. Lingyi Meng, Yu Zhang and **ChiYung Yam**
Multiscale study of plasmonic scattering and light trapping effect in silicon nanowire array solar cells
J. Phys. Chem. Lett. 2017, 8, 571-575

30. Saranya Govindarajan, Shiwu Gao, Wei Cai and **ChiYung Yam**
Rational design and first-principles studies of phenothiazine-based dyes for dye-sensitised solar cells
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31. Rulin Wang, Yu Zhang, Fuzhen Bi, Thomas Frauenheim, GuanHua Chen and **ChiYung Yam**
Quantum mechanical modeling the emission pattern and polarization of nanoscale light emitting diodes
Nanoscale 2016, 8, 13168-13173 (Back Cover)

32. Yu Zhang, **ChiYung Yam** and George C. Schatz
Fundamental limitations to plasmonic hot-carrier solar cells
J. Phys. Chem. Lett. 2016, 7, 1852-1858

33. Bang-Ming Ming, Ru-Zhi Wang, **ChiYung Yam**, Li-Chun Xu, Woon-Ming Lau and Hui Yan
Bandgap engineering of GaN nanowires
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34. Jianping Xiao, Liangzhi Kou, **ChiYung Yam**, Thomas Frauenheim and Binghai Yan
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ACS Catal. 2016, 5, 7063-7067

35. Lingyi Meng, **ChiYung Yam**, Yu Zhang, Rulin Wang and GuanHua Chen
Multiscale modeling of plasmon-enhanced power conversion efficiency in nanostructured solar cells
J. Phys. Chem. Lett. 2015, 6, 4410-4416

36. Rulin Wang, Xiao Zheng, YanHo Kwok, Hang Xie, GuanHua Chen and **ChiYung Yam**
Time-dependent density functional theory for open systems with a positivity-preserving decomposition scheme for environment spectral functions
J. Chem. Phys. 2015, 142, 144112

37. Rulin Wang, Yu Zhang, GuanHua Chen and **ChiYung Yam**
Quantum mechanical modeling of electron-photon interactions in nanoscale devices
Prog. Electromagn. Res. 2015, 154, 163-170

38. Chuan-Jia Tong, Wei Geng, Zhen-Kun Tang, **ChiYung Yam**, Xiao-Li Fan, Jiang Liu, Woon-Ming Lau and Li-Min Liu
Uncovering the veil of the degradation in perovskite $CH_3NH_3PbI_3$ upon humidity exposure: a first-principles study
J. Phys. Chem. Lett. 2015, 6, 3289-3295

39. Quan Chen, Jun Li, **ChiYung Yam**, Yu Zhang, Ngai Wong and GuanHua Chen
An approximate framework for quantum transport calculation with model order reduction
J. Comp. Phys. 2015, 286, 49-61

40. Yu Zhang, **ChiYung Yam**, YanHo Kwok and GuanHua Chen
A variational approach for dissipative quantum transport in a wide parameter space
J. Chem. Phys. 2015, 143, 104112

41. Yu Zhang, **ChiYung Yam** and GuanHua Chen
Dissipative time-dependent quantum transport theory: quantum interference and phonon induced decoherence dynamics
J. Chem. Phys. 2015, 142, 164101

42. **ChiYung Yam**, Lingyi Meng, Yu Zhang and GuanHua Chen
Multiscale quantum mechanics/electromagnetics method for device simulations
Chem. Soc. Rev. 2015, 44, 1763

43. Stanislav Markov, Balint Aradi, **ChiYung Yam**, Hang Xie, Thomas Frauenheim and GuanHua Chen
Atomic level modeling of extremely thin silicon-on-insulator MOSFETs including the silicon dioxide: Part I – Electronic Structure
IEEE Trans. Electron Dev. 2015, 62, 696-704

44. Hongping Yang, **ChiYung Yam**, Aihua Zhang, Zhiping Xu, Jun Luo and Jing Zhu
Discriminative modulation of the highest occupied molecular orbital energies of graphene and carbon nanotubes induced by charging
Phys. Chem. Chem. Phys. 2015, 17, 7248-7254

45. ShuGuang Chen, Yu Zhang, SiuKong Koo, Heng Tian, **ChiYung Yam**, GuanHua Chen and Mark A. Ratner
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J. Phys. Chem. Lett. 2014, 5, 2748-2752

46. Yu Zhang, LingYi Meng, **ChiYung Yam** and GuanHua Chen
Quantum-mechanical prediction of nanoscale photovoltaics
J. Phys. Chem. Lett. 2014, 5, 1272-1277

47. **ChiYung Yam** and GuanHua Chen
Linear-scaling computation of excited states in time-domain
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48. Jun Z. Huang, Lining Zhang, Weng Cho Chew, **ChiYung Yam**, Li Jun Jiang, GuanHua Chen and Mansun Chan
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49. Lingyi Meng, Zhenyu Yin, **ChiYung Yam**, SiuKong Koo, Quan Chen, Ngai Wong and GuanHua Chen
Frequency-domain multiscale quantum mechanics/electromagnetics simulation method
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50. YanHo Kwok, Hang Xie, **ChiYung Yam**, Xiao Zheng and GuanHua Chen
Time-dependent density functional theory quantum transport simulation in non-orthogonal basis
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51. Jianqiao Zhang, ZhenYu Yin, Xiao Zheng, **ChiYung Yam** and GuanHua Chen
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52. Jun Z. Huang, Weng Cho Chew, Jie Peng, **ChiYung Yam**, Li Jun Jiang and GuanHua Chen
Model order reduction for multiband quantum transport simulations and its application to p-type junctionless transistors
IEEE Trans. Electron Dev. 2013, 60, 2111-2119

53. **ChiYung Yam**, Jie Peng, Quan Chen, Stanislav Markov, Jun Z. Huang, Ngai Wong, Weng Cho Chew and GuanHua Chen
A multi-scale modeling of junctionless field-effect transistors
Appl. Phys. Lett. 2013, 103, 062109

54. Yu Zhang, **ChiYung Yam** and GuanHua Chen
Dissipative time-dependent quantum transport theory
J. Chem. Phys. 2013, 138, 164121

55. Hang Xie, Feng Jiang, Heng Tian, Xiao Zheng, Yanho Kwok, Shuguang Chen, **ChiYung Yam**, YiJing Yan and Guanhua Chen
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56. **ChiYung Yam**, Qing Zhang, Fan Wang and GuanHua Chen
Linear-scaling quantum mechanical methods for excited states
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57. Lingyi Meng, **ChiYung Yam**, SiuKong Koo, Quan Chen, Ngai Wong and GuanHua Chen
Dynamic multiscale quantum mechanics/electromagnetics simulation method
J. Chem. Theory Comput. 2012, 8, 1190-1199

58. SiuKong Koo, **ChiYung Yam**, Xiao Zheng and GuanHua Chen
First-principles Liouville–von Neumann equation for open systems and its applications
Phys. Status Solidi B 2012, 249, 270-275

59. Yong Wang, **ChiYung Yam**, Thomas Frauenheim, GuanHua Chen and Thomas Niehaus
An efficient method for quantum transport simulations in the time domain
Chem. Phys. 2011, 391, 69-77

60. Fan Wang, **ChiYung Yam**, Lihong Hu and GuanHua Chen
Time-dependent density functional theory based Ehrenfest dynamics
J. Chem. Phys. 2011, 135, 044126

61. **ChiYung Yam**, Xiao Zheng, GuanHua Chen, Yong Wang, Thomas Frauenheim and Thomas Niehaus
Time-dependent versus static quantum transport simulations beyond linear response
Phys. Rev. B 2011, 83, 245448

62. Yan Wang, **ChiYung Yam**, Ya Kun Chen and GuanHua Chen
Communication: Linear-expansion shooting techniques for accelerating self-consistent field convergence
J. Chem. Phys. 2011, 134, 241103

63. Shizheng Wan, SiuKong Koo, **ChiYung Yam**, Xiao Zheng, Yijing Yan, Zhongming Su, Kangnian Fan, Li Cao, Wenping Wang and GuanHua Chen
Time-dependent current distributions of a two-terminal carbon nanotube-based electronic device
J. Phys. Chem. B 2011, 115, 5519-5525

64. **ChiYung Yam**, Lingyi Meng, GuanHua Chen, Quan Chen and Ngai Wong
Multiscale quantum mechanics/electromagnetics simulation for electronic devices
Phys. Chem. Chem. Phys. 2011, 13, 14365-14369

65. Xiao Zheng, **ChiYung Yam**, Fan Wang and GuanHua Chen
Existence of time-dependent density-functional theory for open electronic systems: Time-dependent holographic electron density theorey
Phys. Chem. Chem. Phys. 2011, 13, 14358-14364

66. Xiao Zheng, GuanHua Chen, Yan Mo, SiuKong Koo, Heng Tian, **ChiYung Yam** and Yijin Yan
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67. JianZhou Zheng, Xiao Zheng, **ChiYung Yam** and GuanHua Chen
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70. Binghai Yan, **ChiYung Yam**, Andreia Luisa da Rosa and Thomas Frauenheim
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71. **ChiYung Yam**, Yan Mo, Fan Wang, Xiaobo Li, GuanHua Chen, Xiao Zheng, Yuki Matsuda, Jamil Tahir-Kheli and William A. Goddard III
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72. Fan Wang, **ChiYung Yam**, GuanHua Chen, XiuJun Wang, Kangnian Fan, Thomas A. Niehaus and Thomas Frauenheim
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73. Fan Wang, **ChiYung Yam** and GuanHua Chen
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74. Xiao Zheng, Fan Wang, **ChiYung Yam**, Yan Mo and GuanHua Chen
Time-dependent density-functional theory for open systems
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75. Fan Wang, **ChiYung Yam** and GuanHua Chen
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76. JianZhou Zheng, Xiao Zheng, Yang Zhao, Yang Xie, **ChiYung Yam**, GuanHua Chen, Qing Jiang and Allen T. Chwang
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77. **ChiYung Yam**, Xiao Zheng and GuanHua Chen
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79. ChiChiu Ma, Yang Zhao, **ChiYung Yam**, GuanHua Chen and Qing Jiang
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80. **ChiYung Yam**, ChiChiu Ma, XiuJun Wang and GuanHua Chen
Electronic structure and charge distribution of potassium iodide intercalated single walled carbon nanotubes
Appl. Phys. Lett. 2004, 85, 4484-4486

81. **ChiYung Yam**, Satoshi Yokojima and GuanHua Chen
Localized-density-matrix implementation of time-dependent density-functional theory
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82. **ChiYung Yam**, Satoshi Yokojima and GuanHua Chen
Linear-scaling time-dependent density-functional theory
Phys. Rev. B 2003, 68, 153105