CURRICULUM VITAE

Name: GuanHua Chen

Present position: Professor, Department of Chemistry, The University of Hong Kong

Education:

- **Ph.D.** (5/92): Physics, California Institute of Technology **(*Advisor:*** William A Goddard III**)**
- **B. S.** (6/86): Physics, Fudan University, China

Academic Positions:

- Professor, Department of Chemistry, HKU 09/2006-Present
- Head, Department of Chemistry, HKU 05/2010-05/2016
- Associate Professor Department of Chemistry, HKU 12/1999-08/2006
- Assistant Professor Department of Chemistry, HKU 07/1996-11/1999
- Postdoctoral Fellow Department of Chemsitry, University of Rochester 07/1993– 02/1996
  (Advisor: Shaul Mukamel**)**

Honorary Positions:

- Guest Professor, University of Science and Technology of China (2005-);
- Adjunct Professor, Zhongshan University (2002-2005);
- Adjunct Professor, Dalian Institute of Chemical Physics (2002-2006);
- Guest Professor, Northeast Normal University(1999-);
- Senior Visiting Scholar, Fudan University (2003-2005)
- Senior Visiting Scholar, Tsinghua University (2005-2011)

Awards:

- Croucher Senior Research Fellowship (2016)
- Outstanding Young Scholar Award, NSFC (2009-2010)
- National Natural Science Award (First Class), Education Ministry of China (2008)
- Outstanding Young Researcher Award 2001-2002, The University of Hong Kong
- Co-1st place in China-US Physics Examination and Application (CUSPEA) program (1985)

Professional Services / Standing:

- Fellow of American Physical Society (2014-)
- Fellow of Royal Chemical Society (2011-)
- Vice-President of Hong Kong Institution of Science (2013-2015)
- Editorial Board, Journal of Physical Chemistry (2017-)

- ❖ Editor Board, Journal of Physical Chemistry Letters (2017-)
- ❖ Associate Editor, European Physical Journal B (2012-2017)

Organizing Conferences

1. Conference organizer, "Workshop on Quantum Simulation", Dec 8th, 2014, Hong Kong
2. Conference co-organizer, "The Workshop on Simulation and Modeling of Emerging Electronics 2014", Dec 15-16th, 2014, Hong Kong
3. Conference organizer, "Workshop on Computational Materials and Computational Biology", Nov 6-7th, 2014, Hong Kong
4. Conference organizer, "Hong Kong Spring School on Quantum Simulation Methods", April 7-11th, 2014, Hong Kong
5. Conference organizer, "Hong Kong Workshop in Computer Modeling of Complex Processes (CMCP)", Dec 17-19th, 2013, Hong Kong
6. Conference co-organizer, "Workshop on Simulation and Modeling of Emerging Electronics 2013", Dec 18-20th, 2013, Hong Kong
7. Conference organizer, "Hong Kong Workshop on Dynamics of Molecules and Materials", Dec 16th, 2013, Hong Kong
8. Conference organizer, "The 21st Annual Conference of Hong Kong Institution of Science" Nov 23rd, 2013, Hong Kong
9. Conference organizer, "2013 HKU Workshop on Computational Science and Engineering", Jun 21, 2013, Hong Kong
10. Conference organizer, "Workshop on Computational Methods for Complex Systems", Dec 9-12th, 2012, Hong Kong
11. Conference organizer, "CECAM Workshop on Simulation and Modeling of Emerging Electronics", Dec 12-16th, 2011, Hong Kong
12. Conference organizer, "International Workshop on Simulation and Modeling of Emerging Electronics", Dec 6-10th, 2010, Hong Kong
13. Conference Co-organizer, "One-Dimensional nano-materials: Performance, Devices and NEMS International Workshop", Jun 26-29th, 2007. Nanchang, P. R. China
14. Conference Co-organizer, "International Workshop on Computational Methods for Nanoscale Systems", Dec 11-13rd, 2006, Hong Kong
15. Conference Co-organizer, "International Workshop on Theoretical and Computational Chemistry of Complex Systems in conjunction with 3rd Chinese Theoretical and Computational Chemistry Conference", Jan 3-7th, Hong Kong

Research Outputs / Publications

1. "STM Imaging of Electron Migration in Real Space and Time: A Simulation Study", Y.H. Kwok, **G.H. Chen**, S. Mukamel, Nano Lett. 2019, 19, 7006-7012.
2. "Efficient Corrections for DFT Noncovalent Interactions Based on Ensemble Learning Models", W.Z. Li, W. Miao, J.X. Cui, C. Fang, S.T. Su, H.Z. Li. L.H. Hu, Y.H. Lu, **G.H. Chen**, J. Chem. Inf. Model. 2019, 59, 1849-1857.

3. "Fundamental Limit to Scaling Si Field-Effect Transistors Due to Source-to-Drain Direct Tunneling", S. Markov, Y.H. Kwok, J. Li, W.J. Zhou, Y. Zhou, **G.H. Chen**, IEEE Trans. Electron Devices 2019, 66, 1167-1173.
4. "First principles investigation of the surface stability and equilibrium morphology of MoO_3", S.P. Sun, J.L. Zhu, S. Gu, X.P. Li, W.N. Lei, Y. Jiang, D.Q. Yi, **G.H. Chen**, Appl. Surf. Sci. 2019, 467, 753-759.
5. "Stark control of electrons along nanojunctions", L. Chen, Y. Zhang, **G.H. Chen**, I. Franco, Nat. Comm. 2018, 9, 2070.
6. "Size-independent neural networks based first-principles method for accurate prediction of heat of formation of fuels", G.Y. Yang, J. Wu, S.G. Chen, W.J. Zhou, J. Sun, **G.H. Chen**, J. Chem. Phys. 2018, 148, 241738.
7. "Designing Principles of Molecular Quantum Interference Effect Transistors", S.G. Chen, **G.H. Chen**, M.A. Ratner, J. Phys. Chem. Lett. 2018, 9, 2843-2847.
8. "Computing the full spectrum of large sparse palindromic quadratic eigenvalue problems arising from surface Green's function calculations", T.-M. Huang, W.-W. Lin, H. Tian, **G.H. Chen**, J. Comput. Phys. 2018, 356, 340-355.
9. "First principles investigation of the electronic properties of graphitic carbon nitride with different building block and sheet staggered arrangement", S.P. Sun, S. Gu, J.H.Sun, F.F.Xia, **G.H.Chen**, J. Alloys Compd. 2018, 735, 131-139.
10. "Time-Dependent Density Functional Theory for Open Systems and Its Applications", S. G. Chen, Y. H. Kwok, and **G. H. Chen**. Acc. Chem. Res. 2018, 51, 385−393.
11. "Can Molecular Quantum Interference Effect Transistors Survive Vibration?", S. G. Chen, W. J. Zhou, Q. Zhang, Y. H. Kwok, **G. H. Chen**, and M. A. Ratner. *J. Phys. Chem. Lett.* 2017, 8, 5166−5170.
12. "Enhanced Photovoltaic Properties Induced by Ferroelectric Domain Structures in Organometallic Halide Perovskites", F. Z. Bi, S. Markov, R. L. Wang, Y. H. Kwok, W. J. Zhou, L. M. Liu, X. Zheng, **G. H. Chen**, and C. Y. Yam. *J. Phys. Chem. C* 2017, 121, 11151−11158
13. "Structure descriptor for surface passivation in the simulation of atomistic models", L. Cao, S. K. Koo, J. Sun**, G. H. Chen**, W. P. Wang. *Sci China Inf Sci*, 2017, 60(3).
14. "Quantum mechanical modeling the emission pattern and polarization of nanoscale light emitting diodes", R. L. Wang, Y. Zhang, F. Z. Bi, T. Frauenheim, **G. H. Chen** and C. Y. Yam. *Nanoscale*, 2016, 8, 13168–13173 .
15. "Quantum Mechanical Modeling of Electron-Photon Interactions in Nanoscale Devices.", R. L. Wang, Y. Zhang, **G. H. Chen**, C. Y. Yam. *Progress In Electromagnetics Research* 154 (2015): 163-170.
16. "Permittivity of Oxidized Ultra-Thin Silicon Films From Atomistic Simulations.", S. Markov, G. Penazzi, Y. H. Kwok, A. Pecchia, B. Aradi., T. Frauenheim, **G. H. Chen**. *IEEE Electron Device Lett*. 2015, 36 (10), 1076-1078.
17. "Multiscale Modeling of Plasmon-Enhanced Power Conversion Efficiency in Nanostructured Solar Cells", L.Y. Meng, C. Y. Yam, Y. Zhang, R. L. Wang, and **G. H. Chen**. *J. Phys. Chem. Lett.* 6 (2015) : 4410-4416 .
18. "A variational approach for dissipative quantum transport in a wide parameter space", Y. Zhang, C. Y. Yam, Y. H. Kwok, **G. H. Chen.** *J. Chem. Phys.* 143, 104112 (2015).
19. "MAGEA10 gene expression in non-small cell lung cancer and A549 cells, and the affinity of epitopes with the complex of HLA-A*0201 alleles", L. K. Wang, Y. F. Xu, C. Luo, J. Sun, J. L. Zhang, M. W. Lee, A. P. Bai, **G. H. Chen**, C. M. Frenz, Z.G. Li, W.L. Huang, Cell. Immunol. (2015).

20. "Dissipative time-dependent quantum transport theory: Quantum interference and phonon induced decoherence dynamics", Y. Zhang, C. Y. Yam, **G. H. Chen**, *J. Chem. Phys.* 142, 164101 (2015).
21. "Time-dependent density functional theory for open systems with a positivity-preserving decomposition scheme for environment spectral functions", R.L. Wang, X. Zheng, Y. H. Kwok, H. Xie, **G. H. Chen**, C. Y. Yam*, J. Chem. Phys.* 142, 144112 (2015).
22. "What are Memristor, Memcapacitor, and Meminductor?", Z.Y. Yin, H. Tian, **G. H. Chen**, L. O. Chua, *IEEE Trans. Circ. Syst. II*, 62, 402 (2015). DOI:10.1109/TCSII.2014.2387653
23. "Atomic Level Modeling of Extremely Thin Silicon-on-Insulator MOSFETs Including the Silicon Dioxide: Electronic Structure", S. Markov, B. Aradi, C. Y. Yam, H. Xie, T. Frauenheim, **G. H. Chen**, *IEEE Trans. Elec. Dev*., 62, 696 (2015). DOI:10.1109/TED.2014.2387288
24. "An approximate framework for quantum transport calculation with model order reduction", Q. Chen, J. Li, C. Y. Yam, Y. Zhang, N. Wong, **G. H. Chen**, *J. Comp. Phys.,* 286, 49-61 (2015). DOI:10.1016/j.jcp.2015.01.032
25. "A multiscale quantum mechanics/electromagnetics method for device simulations", C. Y. Yam, L.Y. Meng, Y. Zhang, **G. H. Chen**, *Chem. Soc. Rev*. 44, 1763 (2015). DOI:10.1039/c4cs00348a
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28. "Alternative Approach to Chemical Accuracy: A Neural Networks-Based First-Principles Method for Heat of Formation of Molecules Made of H, C, N, O, F, S, and Cl", J. Sun, J. Wu, T. Song, L.H. Hu, K.L. Shan, **G. H. Chen**, J. *Phys. Chem. A* (2014).
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33. "Time-dependent density functional theory quantum transport simulation in non-orthogonal basis", Y. H. Kwok, H. Xie, C. Y. Yam, X. Zheng, **G. H. Chen**, *J. Chem. Phys.* 139, 224111 (2013).
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35. "Linear-scaling computation of excited states in time-domain", C. Y. Yam, **G. H. Chen**, Sci. China Chem., 57, 70-77, (2013). DOI:10.1007/s11426-013-5007-5
36. "Gauge-invariant and current-continuous microscopic ac quantum transport theory", J.Q. Zhang, Z.Y. Yin, X. Zheng, C. Y. Yam, **G. H. Chen**, *Eur. Phys. J. B* 86, 423, (2013).
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40. "Time-dependent density functional theory for quantum transport", Y. H. Kwok, Y. Zhang, **G. H. Chen**, *Front. Phys.* (2013).
41. "Model Order Reduction for Multiband Quantum Transport Simulations and its Application to p-Type Junctionless Transistors", J. Z. Huang, W. C. Chew, J. Peng, C. Y. Yam, L. J. Jiang, **G. H. Chen**, *IEEE Trans. on Elec. Dev.* Vol. 60, No. 7, 2111-2119 (2013).
42. "A multi-scale framework for nano-electronic devices modeling with application to the junctionless transistor", J. Peng, Q. Chen, N. Wong, L.Y. Meng, C. Y. Yam, **G. H. Chen**, IEEE International Conference of Electron Devices and Solid-State Circuits (EDSSC), P.1-2 (2013). DOI:10.1109/EDSSC.2013.6628145
43. "A Numerically Efficient Formulation for Time-Domain Electromagnetic-Semiconductor Cosimulation for Fast-Transient Systems", Q. Chen, W. Schoenmaker, **G. H. Chen**, L.J. Jiang, N. Wong, *IEEE Trans. on CAD of IC and Sys.* Vol. 32, No. 5, 802-806 (2013).
44. "Dissipative time-dependent quantum transport theory", Y. Zhang, C. Y. Yam, **G. H. Chen**, *J. Chem. Phys.* 138, 164121 (2013).
45. "Theoretical insights into [PMo12O40](3-) grafted on single-walled carbon nanotubes", S.Z. Wen, W. Guan, Y.H. Kan, G.C. Yang, N.N. Ma, L.K. Yan, Z.M. Su, **G. H. Chen**, *Phys. Chem. Chem. Phys.* 15, 9177 (2013).
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48. "Quantum transport through an array of quantum dots", S.G. Chen, H. Xie, Y. Zhang, X.D. Cui, and **G. H. Chen**, *Nanoscale* 5, 169 (2013).
49. "Time-dependent quantum transport: An efficient method based on Liouville-von-Neumann equation for single-electron density matrix", H. Xie, F. Jiang, H. Tian, X. Zheng, Y. H. Kwok, S.G. Chen, C. Y. Yam, Y. J. Yan, and **G. H. Chen**, *J. Chem. Phys.* 137, 044113 (2012).
50. "Quantum Transport Simulations Based on Time Dependent Density Functional Theory", Thomas Niehaus and **Guanhua Chen**, Chapter 2 of "*Quantum Simulations of Materials and Biological Systems*", p.17-32, Ed. Jun Zeng, Rui-Qin Zhang, Herbert R. Treutlein, Springer (2012).
51. "Dynamic Multiscale Quantum Mechanics/Electromagnetics Simulation Method", L.Y. Meng, C. Y. Yam, S. K. Koo, Q. Chen, N. Wong and **G. H. Chen**, *J. Chem. Theory Comput.* 8, 1190 (2012).
52. "First-principles Liouville-von Neumann equation for open systems and its applications", S. K. Koo, C. Y. Yam, X. Zheng and **G. H. Chen**, Phys. Status Solidi B, 249, 270 (2012). DOI:10.1002/pssb.201100530
53. "Structure-dependent optical properties of single-walled silicon nanotubes", M. Zhang, Z.M. Su and **G. H. Chen**, *Phys. Chem. Chem. Phys.* 14, 4695 (2012).
54. "Linear-scaling quantum mechanical methods for excited states", C.Y. Yam, Q. Zhang, F. Wang and **G. H. Chen**, *Chem. Soc. Rev.* 41, 3821 (2012).
55. "Sequential Establishment of Stripe Patterns in an Expanding Cell Population", C.L. Liu, X.F. Fu, Liu, L.Z. Liu, Xiaojing Ren,; Carlos K. L. Chau, Sihong Li, Lu Xiang, Hualing Zeng, **Guanhua Chen**, Lei-Han Tang, Peter Lenz, Xiaodong Cui, Wei Huang, Terence Hwa, and Jian-Dong Huang, *Science* 334, 238 (2011).
56. "Time-dependent density functional theory based Ehrenfest dynamics", F. Wang, C.Y. Yam, L.H. Hu, **G. H. Chen**, *J. Chem. Phys.* 135, 044126 (2011).
57. "Time-dependent versus static quantum transport simulations beyond linear response", C. Y. Yam, X. Zheng, **G. H. Chen**, Y. Wang, T. Frauenheim, T. A. Niehaus, *Phys. Rev. B* 83, 245448 (2011).
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59. "Time-Dependent Current Distributions of a Two-Terminal Carbon Nanotube-Based Electronic Device", S. Z. Wen, S. K. Koo, C. Y. Yam, X. Zheng, Y. J. Yan, Z. M. Su, K. N. Fan, L. Cao, W. P. Wang, **G. H. Chen**, *J. Phys. Chem. B* 115, 5519-5525 (2011).
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63. "Time-dependent versus static quantum transport simulations beyond linear response" ChiYung Yam, Xiao Zheng, **GuanHua Chen**, Yong Wang, Thomas Frauenheim, and Thomas A. Niehaus, *Phys. Rev. B* 83, 245448 (2011).
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Plenary/Keynote Lectures:

1. "Quantum mechanical simulation of transient currents through molecular devices", *The 9th International Conference on Computational Physics (ICCP9)*, Jan 7-11, 2015, Singapore
2. "Quantum mechanical simulation of open electronic systems: from molecular device to semiconductor transistor", June 12-15, 2014, Taiyuan, China
3. "Combined first-principles calculation and Neural Networks Correction Approach for Heat of Formation", *International Conference on Pure and Applied Chemistry 2012*, July 2-6, 2012, Mauritius.
4. "First-principles method for open systems", *International Workshop on One-Dimensional Nanostructured Materials: Properties, Devices and NEMS*, June 25-28, 2007, Nanchang, China.
5. "Combined first-principles calculation and Neural Network correction approach as a powerful tool in computational physics and chemistry", *The First International Conference on Theoretical Chemistry, Molecular Modeling and Life Sciences,* Aug. 17-20, 2003, Beijing, China
6. "Quantum mechanical simulation for nanoscopic materials", *Annual meeting of the frontier theoretical physics and related fields,* Jan. 15-17, 2003, Beijing.
7. "Quantum Mechanical Simulation of Nanomaterials and Macromolecules", *8th National Conference on Quantum Chemistry*, July 17-22, 2002, Changchun, China

Invited Lectures:

1. The international chemical congress of pacific basin societies 2015, Honolulu, Hawaii, US, Dec 15-20, 2015
2. 2015 Shanghai International Symposium on Computational Chemistry, Shanghai, China, Aug 23-26, 2015
3. Quantum Transport in Nanoscale Molecular Systems, Colorado, USA, July 20-24, 2015
4. The Batsheva de Rothschild seminar on molecular electronics 2015, Israel, Jun 7-12, 2015
5. 5th Chinese-French Workshop in Theoretical Chemistry, Strasbourg, France, May 10-13
6. "TD-DFT for quantum transport and beyond", Perspectives of many- particle methods: Total energy, spectroscopy and time-dependent dynamics, Bremen, Germany, April 20-24, 2015
7. "Time-dependent simulation of open systems", Quantum Effects in Biological Systems Workshop 2014, Singapore, Dec 2-5, 2014
8. "Quantum mechanical simulation of open electronic systems: from molecular devices to photovoltaics", 19th International Workshop on Quantum Systems in Chemistry, Physics and Biology, Taipei, Nov11-17, 2014
9. Current Topics in Theoretical Chemistry, Nha Trang, Vietnam, Aug 25-29, 2014

10. “Time-Dependent Density-Functional Theory for Open System”, the Workshop on Excited States and Time-dependent Electronic Structure Theory, Colorado, USA, Jul 14-18, 2014
11. “Quantum mechanical simulation of open electronic systems: from molecular devices to grapheme”, the 26th Canadian Symposium on Theoretical and Computational Chemistry (CSTCC), Montreal, Canada, Jul 6-11, 2014
12. “Quantum Mechanical Simulation of Nanoscale Photovoltaic Devices”, the 2014 Conference on Excited State Processes, Los Alamos, USA, Jun 9-12, 2014
13. “Quantum mechanical simulation of open electronic systems: from molecular device to semiconductor transistor”, The 12th National Conference of Quantum Chemistry of China (NCQC), Taiyuan, China, Jun 15-20, 2014
14. “Molecular Motor”, 2013 Hong Kong Workshop in Computer Modeling of Complex Processes, Hong Kong, Dec 17-19, 2013
15. “First-principles and Multiscale Simulations of Emerging Electronics”, The Workshop on Simulation and Modeling of Emerging Electronics 2013, Dec 18-20, 2013
16. “Multiscale simulation of junctionless transistor”, International Workshop on Computational Science and Engineering 2013, National Taiwan University, Oct. 16, 2013.
17. “Holding infinity in the palm of your hand: *from holographic electron density theorem to first-principles method for open systems*”, July 31, 2013, California Institute of Technology, Pasadena, USA.
18. “An Alternative Approach to Chemical Accuracy”, Walailak University, Thailand, Oct. 28, 2013.
19. “Interference and Molecular Transport: Time-dependent Analysis of Disubstituted Benzenes”, Telluride workshop on Nonequilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy, July 22-26, 2013, Colorado, USA.
20. “Holding infinity in the palm of your hand: *from holographic electron density theorem to first-principles method for open systems*”, 6th APCTCC, South Korea, July 11, 2013.
21. “Time-dependent quantum transport through metallic wires”, CACAM Workshop "Molecular electronics: Quo vadis?", Univ. Bremen, Bremen, Germany, March 4-8, 2013.
22. “QM/EM method and its application”, *International Symposium on Computics: Quantum Simulation and Design (ISC-QSD)*, Osaka, Japan, October 11 - 13, 2012
23. “Multiscale Simulation of Emerging Electronics”, *Telluride Workshop on Nanomaterials - Theory and Computation*, Telluride, Colorado, USA, July 16-20, 2012.
24. “Penetrating a potential barrier one hundred percent”, *Kathmandu 2012 Workshop on Theoretical Chemistry- Atoms, molecules and solids: models and concepts*, Kathmandu, Apr 30–May 4, 2012.
25. "Towards first-principles simulation of transient currents through molecular and nanoscopic devices", *15th International Workshop on Computational Electronics (IWCE 2012)*, University of Wisconsin – Madison, May 22-25, 2012.
26. “QM/EM simulation of emerging electronics”, the 9th Cross-Strait Workshop on Nano Science and Technology, National Cheng Kung University, Tainan, Taiwan, April 22-25, 2012.
27. “Towards first-principles simulation of transient currents”, *CECAM Workshop on Simulation and Modeling of Emerging Electronics*, University of Hong Kong, Hong Kong, Dec. 12-16, 2012.
28. “Time-dependent density-functional theory for open system”, *CECAM Workshop on Perspectives and Challenges of Many-Particle Methods*, University of Bremen, Bremen, Germany, Sep. 19-23, 2011.
29. Telluride Workshop on non-equilibrium phenomena, nonadiabatic dynamics and spectroscopy, Telluride, Colorado, USA, July 4-8, 2011.

30. "*First-principles quantum kinetic equation for transport"*, Workshop on Quantum Transport and Nanoelectronics, Renmin University, Beijing, Aug. 11-13, 2011.
31. "Multiscale Quantum Mechanics/Electromagnetics Simulation of Emerging Electronics", *First Summer School on Quantum Transport Simulation*, Beijing, Aug. 15-19, 2011.
32. "First-principles Liouville-von Neumann Equation for Open System", *DICP Symposium on Theoretical and Computational Chemistry*, Dalian Institute of Chemical Physics, Dalian, China, Aug. 16-19, 2011.
33. "First-principle methods for open systems and multiscale simulation of emerging electronics", Jilin University, Jilin, China, April 7, 2010.
34. "Time-dependent density-functional theory for open systems and its application to emerging electronics", 5th World-wide Chinese Theoretical Chemist Conference, Xiamen, December 13-17, 2009.
35. "Transient current through Carbon Nanotube-based Molecular Electronic Devices and Their Equivalent Electric Circuit", International CECAM-Workshop "Quantum transport on the molecular scale" Bremen Center for Computational Materials Science University of Bremen, Germany, September 14 – 18, 2009.
36. "First-principles simulation of transient currents through molecular devices", 7th Cross-Strait Workshop on Nanoscience and Nanotechnology, Guizhou, China, July 26-Aug. 1, 2009.
37. "First-principles method for open systems and its application", 3rd cross-strait theoretical and computational chemistry conference, Chengdu, China, April 23-26, 2009.
38. "First-principles method for open systems and its application", Life in Liouville Space: 30 years of Theoretical Spectroscopy—Symposium in Honor of Shaul Mukamel", University of California, Irvine, USA, Dec. 15-16,2008.
39. "Dynamic Admittance of Carbon Nanotube-based Molecular Electronic Devices and Their Equivalent Electric Circuit", AsiaNANO 2008, Nov. 3-6, 2008, Singapore.
40. "O(N) time-dependent density-functional theory", ICCMSE 2008, Sep. 26-30, 2008, Iraklion, Crete, Greece.
41. "Time-dependent density-functional theory for open systems and its application to molecular electronics", 2008 International Workshop on Frontiers of Theoretical and Computational Physics and Chemistry, July 26-28, 2008, Hohhot, China.
42. "Time-Dependent Density-Functional Theory for Open System and Its Application to Molecular Electronics", 6th Congress of the International Society for Theoretical Chemical Physics, July 19-24, University of British Columbia, Vancouver, Canada.
43. "Linear-scaling time-dependent density-functional theory", CECAM Workshop on Linear-scaling methods, Sep. 3-6, 2007, Lyon, France.
44. "Time-dependent density-functional theory for open systems and its calculation of transient current through molecular devices", 234th American Chemical Society National Meeting, Boston, USA, Aug. 19-23, 2007
45. "Photophysics of DNA and light harvesting systems", 17th International Conference on Phosphorus Chemistry, Xiamen, China, April 15th to 21st, 2007.
46. "Transient current through molecular devices", gDFTB Workshop, Bremen, Germany, Dec. 1-2, 2006.
47. "First-principles methods for open electronic systems", International Conference of Computational Methods in Science and Engineering 2006 (ICCMSE 2006), Oct. 27 – Nov. 1, 2006, Greece.
48. The 4th Worldwide Chinese Theoretical and Computational Chemistry Conference, Aug. 6-10, 2006, Kunming, China.
49. "First-princples TDDFT for open electronic systems", 2006 International Workshop on Frontiers of Theoretical and Computational Physics and Chemistry, Zhang Jia Jie, China, July 8-9, 2006.

50. “Development of Quantum Chemistry Methods for Complex Systems”, Workshop on Quantum Mechanical Methods, Aug. 3-6, 2006, Shanghai.
51. “First-principles simulations of open systems”, Hong Kong – Japan Workshop on Carbon Nanotubes, April 12-13, 2006, Hong Kong.
52. “Some progresses in DFT: efficiency, accuracy and applicability”, 231st American Chemical Society National Meeting, March 26-30, 2006.
53. “Some progresses in DFT: efficiency, accuracy and applicability”, International Symposium of Theoretical and Computational Chemistry on Complex Systems, Nov. 23-26, 2005, Xiamen, China.
54. “Computer simulation of nanomaterials”, The Third International Union of Pure and Applied Chemistry (IUPAC) New Directions in Chemistry Workshop on Advanced Materials (WAM-III), Sep. 5-8, 2005, Stellenbosch, South Africa.
55. “First-principles simulation of open electronic systems”, Atomistix first conference on atomic scale modeling in nanotechnology, The Niels Bohr Summer Institute on Nanoscience, Aug. 18-19, 2005, Copenhagen, Denmark
56. “Tribological study of carbon nanotube oscillators”, The International Union of Theoretical and Applied Mechanics (IUTAM) Symposium 2005, June 27-30, 2005, Beijing, China.
57. “Linear-scaling method for excited states”, Department of Physics, McGill University, March, 2005.
58. “Optical properties and field emission mechanism of carbon nanotubes”, Pacific Rim Conference in Nano Science, Broome, Western Australia, 7-11 September, 2004.
59. “Tribological study of nanomechanical devices”, Advanced Symposium on Theoretical and Computational Chemistry, Aug. 15-19, 2004, Dalian, China.
60. “Linear-scaling time-dependent Hartree-Fock and time-dependent density-functional theory”, Chemistry Summer School at Peking University, Aug. 1-20, 2004, Beijing.
61. “Linear-scaling quantum mechanical methods for complex systems”, T.-D. Lee Summer School, July 22, Beijing.
62. “Quantum mechanical simulation of field emission of a micrometer-long carbon nanotube”, the 4th Oversea Chinese Physicist Association Conference, Shanghai, June 28-July 2, 2004.
63. “Linear-scaling quantum mechanical method for excited states”, Max-Planck-Institut für Physik Komplexer Systeme, July 15, 2004, Dresden, Germany.
64. “Electric, Optical and Mechanical Properties of Carbon Nanotubes”, Department of Physics, University of Paderborn, July 8, 2004, Paderborn, Germany.
65. “Computer simulation of carbon-nanotube-based electronic, optical and mechanical devices”, 3rd International Conference on Computational Modeling and Simulation of Materials, May 29 - June 4, 2004, Acireale, Sicily, Italy.
66. “Computer simulation of field emission from a micrometer-long carbon nanotube”, March 29, 2004, City University of Hong Kong, Hong Kong, China;
67. “Computer simulation of carbon nanotube field emission and nanomechanical devices”, March 23, 2004, Hong Kong Baptist University, Hong Kong, China;
68. “Electronic and Tribological Properties of Several Carbon Nanotubes”, Symposium on the Physical Properties of Carbon Nanotubes, Jan. 6, 2004, HKUST, Hong Kong, China;
69. “Quantum simulation of excited states in nanoscopic systems”, Excited States Processes in Electronic and Bio Nanomaterials, Aug. 11-16, 2003, Los Alamos, New Mexico, USA;
70. “Optical properties of carbon nanotubes”, Two-day international workshop on carbon rich materials, The University of Hong Kong, Jan. 12-14, 2003;

71. “Universal Absorption-Spectral Features of Single-Walled Carbon Nanotubes”, 2nd Cross-Strait Workshop on Nano Science and Technology, City University of Hong Kong, Hong Kong, Dec. 9-11, 2002;
72. “Low-lying Excitations of Light Harvesting System II”, The Hong Kong University of Science and Technology, Dec. 6, 2002;
73. “Optical Properties of Carbon Nanotubes”, Baptise University of Hong Kong, Nov. 5, 2003;
74. “Optical Properties of Single-Walled Carbon Nanotubes”, Yangtze Conference of Fluids and Interfaces, Nanjing, China, Oct. 12-18, 2002;
75. “Optical Properties of Single-Walled Carbon Nanotubes”, National Central University, Taiwan, Sep. 5, 2002;
76. “Quantum Mechanical Simulation of Nano-materials and Macromolecules”, World-wide Chinese Theoretical and Computational conference (WCTCC) 2002, Taipei, Sep. 2-7, 2002;
77. “Linear-scaling quantum chemistry method for excited states: Localized-density-matrix method”, Emerging Technologies in Computational Chemistry Symposium, 224th ACS National Meeting, Boston, Aug. 18-22, 2002;
78. “Localized-density-matrix method: a quantum chemistry method for nanotechnology”, MSC 2001, March 29-30, 2001, California Institute of Technology, USA;
79. “Linear Scaling Quantum Mechanical Calculation of Nano-size Systems”, March 3, Chinese University of Hong Kong, Hong Kong, China;
80. “Simulation of Nanomaterials”, The Third Conference for Worldwide Chinese Young Chemists, Dec. 20-23, 2000, Xiamen, China;
81. “Quantum chemistry simulation of nanomaterials”, Workshop on Condensed Matter Physics, Dec. 17-19, 2000, Zhuhai, China;
82. “Photoexcitations in PPV Aggregates”, International Chinese Workshop on Computational Chemistry, Aug. 14-17, 2000, Dalian, China;
83. “Linear-scaling method for excited states”, MSC 2000, March 23-27, 2000, California Institute of Technology, USA;
84. “Linear-scaling Calculation for Excited State Properties: The Localized-Density-Matrix Method”, Workshop on Computational Chemistry, Feb. 21-23, 2000, Hong Kong University of Science and Technology, Hong Kong;
85. “Intra and inter-chain excitation in PPV aggregates”, Workshop on Light Emitting Materials, Sep. 20, 1999, Fu Jen Catholic University, Taipei, Taiwan;
86. “Linear-scaling localized-density-matrix method and optical properties of carbon nanotubes”, First IUPAC-sponsored Workshop on Advanced Materials, “WAM1: Nanostructured Systems”, July 14-18, 1999, Hong Kong University of Science and Technology, Hong Kong;
87. Workshop on Current Trends in Computer Modeling For Molecular and Material Design, July 12-13, 1999, Chinese University of Hong Kong, Hong Kong;

Research Grants:

1. Development of an accurate and efficient numerical method for quantum transport in time-domain, HK$ 89,600 (PI, G HK701/13, 01/01/2014-31/12/2015)
2. First-principles ac quantum transport theory and its application to carbon nanotube field effect transistors, HK$ 656,521 (PI, GRF, HKU 700913P, 01/01/2014- 31/12/2016)

3. Understanding the coupling of mass-transport and electrochemical reactions in the nanostructured fuel cell electrodes, HK$ 250,000 (Co-I, CRF, HKUST9/CRF/11G, 30/06/2012- 29/06/2015)
4. Quantum mechanical simulation of transient charge transfer in DNA, HK$ 700,000 (PI, GRF, HKU 700912P, 01/01/2013-31/12/2015)
5. Ehrenfest dynamics for open systems and its application to DNA, HK$ 61,000, (PI, Seed Funding Programme for Basic Research, 01/05/2012- 30/04/2014)
6. The development of QM/EM method and its application in the simulation of junction-less FETs, RMB 780,000 (PI, NSFC, 01/01/2013-31/12/2016)
7. Time-dependent density-functional theory for open systems and its application to emerging electronics, HK$ 1,053,000 (PI, RGC, HKU 700711P, 01/01/2012-31/12/2014)
8. Challenges in Organic Photo-Voltaics and Light Emitting Diodes - A Concerted Multi-Disciplinary and Multi-Institutional Effort, HK$ 50,081,000 (Co-I, Theme-based Research Scheme, T23-713/11, 01/01/2012-31/12/2016)
9. Multiscale Quantum Mechanics and Electromagnetics Simulation of Nanoelectronic Devices, HK$ 58,000 (PI, Seed Funding Programme for Applied Research, 201011159085, 01/02/2011-31/01/2013)
10. Electronic design automation software for sub-22nm electronic devices and integrated circuits, HK$ 100,000 (PI, Seed Funding Programme for Applied Research, 201007160005, 01/01/2011-31/12/2011)
11. High frequency response and equivalent circuits of all-graphene electronic devices, HK$ 590,000 (PI, RGC, HKU 700909P, 01/01/2010-31/12/2012)
12. Quantum mechanics / electromagnetics simulation for electronic devices (Co-I, Small Project Funding, 201007176060, 01/09/2010-29/02/2012)
13. Dynamic Response and Equivalent Circuit of Molecular Electronic Devices (Co-I, Seed Funding Programme for Basic Research, 201010159001, 01/12/2010-31/05/2012)
14. **Area of Excellence on Theory, Modeling, and Simulation of Emerging Electronics, HK$ 78,268,000 (PC, AoE/P-04/08, 01/01/2010-31/12/2017)**
15. Experimental and theoretical study of carbon nanotube superconductivity and nanostructured graphene charactistics, HKU 300,000 (Co-PI, Fund Source: CRF; HKUST9/CRF/08;01/03/2009-29/02/2012)
16. Electric properties of molecular electronic devices, 2008-2011, HK$293,700 (Principal Investigator; Fund Source: RGC; HKU 700808P)
17. Fluctuation-driven nanoelectromechanical systems, 2007-2010, HK$267,000 (Principal Investigator; Fund Source: RGC; HKU 701307P)
18. First-principles simulation of dynamic responses of molecular and nanoscopic devices. HK$ 388,460, 2007-09 (Principal Investigator; Fund Source: RGC; HKU 7011/06P)
19. Dynamics of nano bearings, HK$ 250,000, 2007-09 (Co-I; Fund Source: RGC; HKU 7046/06P)
20. Theoretical Investigation of carbon-nanotube-based nanoelectromechanical systems, HK$ 739,300, 2005-08 (Principal Investigator; Fund Source: RGC; N HKU 764/05)
21. Towards the chemical accuracy: combining first-principles methods and Neural Networks, HK$ 308,000, 2006-08 (Principal Investigator; Fund Source: RGC; HKU 7013/05P)
22. Fundamental Study of Nanofluids in Nanochannels of Various Shapes, HK$ 445,784 (Co-I; Fund Source: RGC: HKU 7127/05E)
23. Carbon nanotube/AFI zeolite composite: superconductivity and Li storage application, HK$ 3,500,00, 2005-08 (Co-Investigator; Fund Source: RGC; HKUST 2/04C)

24. Theoretical Investigation and Computer Simulation of Carbon-Nanotube-Based Devices: Gigahertz Oscillators, Field Emitters and Tweezers, HK$ 392,000, 2004-2007 (Principal Investigator; Fund Source: RGC; HKU 7012/04P)
25. Design and Synthesis of Methionine Aminopeptidase-2 Inhibitors as Anti-Angiogenic Agents, HK$ 1,800,000, 2004-2006 (Co-Investigator; Fund Source: RGC; HKU 7359/04M)
26. Towards the first-principles simulation of open systems, HK$ 300,000, 2003-06 (Principal Investigator; Fund Source: RGC; HKU 7010/03P)
27. A first-principles method for calculating STM images of nanoscale molecular systems and its application to alkyl substituted phthalocyanines and porphyrins, HK$ 300,000, 2002-04 (Principal Investigator; Fund Source: RGC; HKU 7099/02P)
28. Photoexcitation in light harvesting systems, HK$ 287,817, 2000-03 (Principal Investigator; Fund Source: RGC; HKU 7100/00P)
29. Linear-scaling semiempirical localized-density-matrix method and photoexcitation in bulk PPV-based materials, HK$ 405,000, 1999-2002 (Principal Investigator; Fund Source: RGC; HKU 7139/99P)
30. Multi-dimensional free energy landscape of a small protein, HK$ 415,000, 1998-2001 (Principal Investigator; Fund Source: RGC; HKU 7093/98P)
31. Dynamics of condensed conjugated materials, HK$ 456,000, 1997-2000 (Principal Investigator; Fund Source: RGC; HKU 7097/97P)

Proceedings of International Conferences：

1. “Electronic Design Automation for sub-20nm Electronics”, International Workshop on Simulation and Modeling of Emerging Electronics, The University of Hong Kong, December, 2010.
2. “Transient current through Carbon Nanotube-based Molecular Electronic Devices and Their Equivalent Electric Circuit”, International CECAM-Workshop “Quantum transport on the molecular scale”, Bremen Center for Computational Materials Science University of Bremen, Germany, September 14 -18, 2009
3. “First-principles simulation of transient currents through molecular devices”, 7th Cross-Strait Workshop on Nanoscience and Nanotechnology, Guizhou, China, July 26-Aug. 1, 2009.
4. “First-principles method for open systems and its application”, 3rd cross-strait theoretical and computational chemistry conference, Chengdu, China, April 23-26, 2009.
5. “First-principles method for open systems and its application”, Life in Liouville Space: 30 years of Theoretical Spectroscopy—Symposium in Honor of Shaul Mukamel”, University of California, Irvine, USA, Dec. 15-16, 2008.
6. “Dynamic Admittance of Carbon Nanotube-based Molecular Electronic Devices and Their Equivalent Electric Circuit”, Asia NANO 2008, Nov. 3-6, 2008, Singapore.
7. “O(N) time-dependent density-functional theory”, ICCMSE 2008, Sep. 26-30, 2008, Iraklion, Crete, Greece.
8. “Time-dependent density-functional theory for open systems and its application to molecular electronics”, 2008 International Workshop on Frontiers of Theoretical and Computational Physics and Chemistry, July 26-28, 2008, Hohhot, China.
9. “Time-Dependent Density-Functional Theory for Open System and Its Application to Molecular Electronics”, 6th Congress of the International Society for Theoretical Chemical Physics, July 19-24, University of British Columbia, Vancouver, Canada.
10. “Linear-scaling time-dependent density-functional theory”, CECAM Workshop on Linear-scaling methods, Sep. 3-6, 2007, Lyon, France.

11. “Time-dependent density-functional theory for open systems and its calculation of transient current through molecular devices”, 234th American Chemical Society National Meeting, Boston, USA, Aug. 19-23, 2007
12. “First-principles method for open systems”, International Workshop on One-Dimensional Nanostructured Materials: Properties, Devices and NEMS, June 25-28, 2007, Nanchang, China.
13. “Photophysics of DNA and light harvesting systems”, 17th International Conference on Phosphorus Chemistry, Xiamen, China, April 15th to 21st, 2007.
14. “Transient current through molecular devices”, gDFTB Workshop, Bremen, Germany, Dec. 1-2, 2006.
15. “First-principles methods for open electronic systems”, International Conference of Computational Methods in Science and Engineering 2006 (ICCMSE 2006), Oct. 27 – Nov. 1, 2006, Greece.
16. The 4th Worldwide Chinese Theoretical and Computational Chemistry Conference, Aug. 6-10, 2006, Kunming, China.
17. “First-principles TDDFT for open electronic systems”, 2006 International Workshop on Frontiers of Theoretical and Computational Physics and Chemistry, Zhang Jia Jie, China, July 8-9, 2006.
18. “Development of Quantum Chemistry Methods for Complex Systems”, Workshop on Quantum Mechanical Methods, Aug. 3-6, 2006, Shanghai.
19. “First-principles simulations of open systems”, Hong Kong – Japan Workshop on Carbon Nanotubes, April 12-13, 2006, Hong Kong.
20. “Some progresses in DFT: efficiency, accuracy and applicability”, 231st American Chemical Society National Meeting, March 26-30, 2006.
21. “Some progresses in DFT: efficiency, accuracy and applicability”, International Symposium of Theoretical and Computational Chemistry on Complex Systems, Nov. 23-26, 2005, Xiamen, China
22. “Computer simulation of nanomaterials”, The Third International Union of Pure and Applied Chemistry (IUPAC) New Directions in Chemistry Workshop on Advanced Materials (WAM-III), Sep. 5-8, 2005, Stellenbosch, South Africa.
23. “First-principles simulation of open electronic systems”, Atomistix first conference on atomic scale modeling in nanotechnology, The Niels Bohr Summer Institute on Nanoscience, Aug. 18-19, 2005, Copenhagen, Denmark
24. “Tribological study of carbon nanotube oscillators”, The International Union of Theoretical and Applied Mechanics (IUTAM) Symposium 2005, June 27-30, 2005, Beijing, China.
25. “Linear-scaling method for excited states”, Department of Physics, McGill University, March, 2005.

Applied Research:

Developed the quantum mechanical simulation software, **LODESTAR**: scientific computing software for quantum simulation of nanoscopic molecular systems and macromolecules

Postgraduate Supervision:

- ❖ Number of Ph.D. candidates under supervision: **7**
- ❖ Number of Ph.D. awarded under my supervision: **22**
- ❖ Number of M.Phil. awarded under my supervision: **2**