CURRICULUM VITAE

Dong-Qing Wei

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Education and Degrees

1987 – 1990 Post-doctoral Fellow, Department of Chemistry, University of British Columbia, Vancouver, B.C., Canada, with Gren Patey.

1985 – 1987 Ph.D., Chemical Physics Program at the Department of Physics, University of Puerto Rico, Rio Piedras, Puerto Rico, USA, thesis supervisor: Lesser Blum.

1982 – 1985 M.S., Department of Chemistry, Normal University of Henan, Xinxiang, Henan, People's Republic of China.

1978 – 1982 B.S., Department of Chemistry, Normal University of Henan, Xinxiang, Henan, People's Republic of China.

Skills & Activities

Computational Biology/Chemistry/Physics: Density Functional Theory, Bioinformatics

Software/Tools/Techniques: Crystal, Ab Initio, Molecular Dynamics Simulation, Ferroelectrics, Lipase, Drug Design, Drug Discovery, Computational Chemistry, QM/MM, Hydrogen Bonding, Autodock, Molecular Mechanics, Molecular Dynamics, Intermolecular Interactions, Molecular Docking, Fluid, Electrolytes, Membrane Proteins, CPMD, Theoretical Chemistry, Cheminformatics and Computational Chemistry, Thermodynamics, Computer Simulations, Apoptosis Assays, Ferroelectric Materials, Free Energy, Phase Transitions, Computational Physics, Biostatistics, Statistical Mechanics, Virtual Screening, Conductivity, Pharmacophore, CSCW, Neuron, Electrostatics, Mutagenesis, Molecular Models, Algebra, Molecular Descriptors, Condensed Matter, Computational Systems Biology, Molecular Modeling, and Correlation.

Languages: English, French, Spanish (Castilian), Chinese

Academic and Research Positions

2006 – Present, Tenured Professor (长聘教授) at the State Key Laboratory of Microbial of Metabolism & Department of Bioinformatics and Biostatistics, College of Life Science and Biotechnology, Shanghai Jiao Tong University, Shanghai, China; an external member at Centre for Research in Molecular Modeling (CERMM), Concordia University in Montreal, Canada; and Adjunct Professor at Pengcheng National Lab.

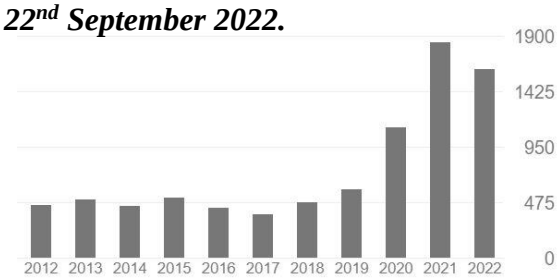
2003-2006, The Haihe Distinguished Professor, appointed by the City of Tianjin at Tianjin Normal University, Directory General, Tianjin Institute of Bioinformatics and Drug Discoveries, Principal Scientist, Gordon Life Science Institute, San Diego, USA, and an external member at Centre for Research in Molecular Modeling (CERMM), Concordia University in Montreal, Canada.
1993 - 2003, Research Scientist, Centre de Recherche en Calcul Applique (CERCA, Research Center on Computation and its Application), Montreal, Quebec.
1990 - 2000, Professor of Chemistry, College of Chemistry and Molecular Engineering, Peeking University, Beijing, P.R. China.
1990 – 1992, Research Associate, Department of Chemistry, University of British Columbia, Vancouver, BC., Canada, with Gren Patey.
1985 – 1985, Assistant Professor, Department of Chemistry, Normal University of Henan, Xinxiang, Henan, People's Republic of China.

Scientific Publications

Publication Performance Metrics 22nd September 2022 by Google Scholar

Citation indices	All	Since 2017
Citations	12428	6067
h-index	61	36
i10-index	252	182

List of Publications (total SCI citations: 12428 times, original papers: 11,018, review and others: 1410) as of 22nd September 2022.



The 15 most significant contributions (cited 2050 times)

1. (Cited 445 times) Chou, K.-C., Wei D.Q., and W.-Z. Zhong, "Binding mechanism of coronavirus main proteinase with ligands and its implication to drug design against SARS". Biochemical and biophysical research communications, 2003. 308(1): p. 148-151.
2. (Cited 347 times) Wei, D. and G. Patey, "Orientational order in simple dipolar liquids: computer simulation of a ferroelectric nematic phase". Physical review letters, 1992. 68(13): p. 2043-2045.
3. (Cited 198 times) Wei, D. and G. Patey, "Ferroelectric liquid-crystal and solid phases formed by strongly interacting dipolar soft spheres". Physical Review A, 1992. 46(12): p. 7783-7792.
4. (Cited 182 times) Sirois, S., Wei D.Q., Q. Du, and K.-C. Chou, "Virtual screening for SARS-CoV protease based on KZ7088 pharmacophore points". Journal of chemical information and computer sciences, 2004. 44(3): p. 1111-1122.

5. (Cited 179 times) Wei, D. and D. Salahub, "Hydrated proton clusters and solvent effects on the proton transfer barrier: A density functional study". The Journal of chemical physics, 1994. 101(9): p. 7633-7642.
6. (Cited 141 times) Wang, J.-F., Wei D.Q., L. Li, S.-Y. Zheng, Y.-X. Li, and K.-C. Chou, "3D structure modeling of cytochrome P450 2C19 and its implication for personalized drug design". Biochemical and biophysical research communications, 2007. 355(2): p. 513-519.
7. (Cited 139 times) Wei, D. and D. Salahub, "Hydrated proton clusters: Ab initio molecular dynamics simulation and simulated annealing". The Journal of chemical physics, 1997. 106(14): p. 6086-6094.
8. (Cited 89 times) Chu, Y., A.C. Kaushik, X. Wang, W. Wang, Y. Zhang, X. Shan, D.R. Salahub, Y. Xiong, and Wei D.Q., "DTI-CDF: a cascade deep forest model towards the prediction of drug-target interactions based on hybrid features". Briefings in Bioinformatics, 2019, DOI: 10.1093/bib/bbz152.
9. (Cited 85 times) Chang, J., P. Lian, Wei D.Q., X.-R. Chen, Q.-M. Zhang, and Z.-Z. Gong, "Thermal decomposition of the solid phase of nitromethane: ab initio molecular dynamics simulations". Physical review letters, 2010. 105(18): p. 188302-188306.
10. (Cited 85 times) Wang, C., Wang, S., Li, D., Wei, D.Q.*, Zhao, J*. and Wang, J.*, "Human intestinal defensin 5 inhibits SARS-CoV-2 invasion by cloaking ACE2". Gastroenterology, 2020, DOI: 10.1053/j.gastro.2020.05.015.
11. (Cited 51 times) Tang, M., Z. Wang, Y. Zhou, W. Xu, S. Li, L. Wang, Wei D.Q., and Z. Qiao, "A novel drug candidate for Alzheimer's disease treatment: gx-50 derived from Zanthoxylum bungeanum". Journal of Alzheimer's Disease, 2013. 34(1): p. 203-213.
12. (Cited 40 times) Gu, R.-X., L.A. Liu, Wei D.Q., J.-G. Du, L. Liu, and H. Liu, "Free energy calculations on the two drug binding sites in the M2 proton channel". Journal of the American Chemical Society, 2011. 133(28): p. 10817-10825.
13. (Cited 34 times) Chu, Y., Shan, X., Chen, T., Jiang, M., Wang, Y., Wang, Q., Salahub, D.R., Xiong, Y. and Wei, D.Q., "DTI-MLCD: predicting drug-target interactions using multi-label learning with community detection method". Briefings in Bioinformatics, 2020, DOI: 10.1093/bib/bbaa205.
14. (Cited 30 times) Wang, Y., D. Hu, and Wei D.Q., "Transmembrane permeation mechanism of charged methyl guanidine". Journal of chemical theory and computation, 2014. 10(4): p. 1717-1726.
15. (Cited 8 times)Chu, Y., Zhang, Y., Wang , Q.K., Zhang, L.F.,Wang, X.H., Wang, Y.J., , Salahub, D.R., Xu, Q.., Wang, J.M., Jiang,X., Xiong, Y*,and Wei, D.Q.*,"A transformer-based model to predict peptide–HLA class I binding and optimize mutated peptides for vaccine design",Nature Machine Intelligence, 2022, 4(3):300-311, DOI: 10.1038/s42256-022-00459-7 (2021).

Other papers listed according to the number of citations (cited 8968 times)

16. (Cited 230 times) Khan, Abbas, et al. "Higher infectivity of the SARS-CoV-2 new variants is associated with K417N/T, E484K, and N501Y mutants: An insight from structural data." *Journal of cellular physiology* (2021), 236(10):7045-7057. doi: 10.1002/jcp.30367.

17. (Cited 141 times) Wei, D.-Q., J.-F. Wang, C. Chen, Y. Li, and K.-C. Chou, "Molecular modeling of two CYP2C19 SNPs and its implications for personalized drug design". Protein and peptide letters, 2008. 15(1): p. 27-32.
18. (Cited 135 times) Blum, L. and Wei D.Q., "Analytical solution of the mean spherical approximation for an arbitrary mixture of ions in a dipolar solvent". The Journal of chemical physics, 1987. 87(1): p. 555-565.
19. (Cited 130 times) Wei, D. and D. Salahub, "A combined density functional and molecular dynamics simulation of a quantum water molecule in aqueous solution". Chemical physics letters, 1994. 224(3-4): p. 291-296.
20. (Cited 126 times) Du, Q., S. Wang, Wei D.Q., S. Sirois, and K.-C. Chou, "Molecular modeling and chemical modification for finding peptide inhibitor against severe acute respiratory syndrome coronavirus main proteinase". Analytical Biochemistry, 2005. 337(2): p. 262-270.
21. (Cited 117 times) Dunbar, R.C., T.B. McMahon, D. Thoelmann, D.S. Tonner, D.R. Salahub, and Wei D.Q., "Zero-pressure thermal-radiation-induced dissociation of gas-phase cluster ions: comparison of theory and experiment for (H2O) 2Cl-and (H2O) 3Cl". Journal of the American Chemical Society, 1995. 117(51): p. 12819-12825.
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25. (Cited 102 times) Wang, S.-Q., Q.-S. Du, K. Zhao, A.-X. Li, Wei D.Q., and K.-C. Chou, "Virtual screening for finding natural inhibitor against cathepsin-L for SARS therapy". Amino Acids, 2007. 33(1): p. 129-135.
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27. (Cited 100 times) Du, Q.-S., S.-Q. Wang, Y. Zhu, Wei D.Q., H. Guo, S. Sirois, and K.-C. Chou, "Polyprotein cleavage mechanism of SARS CoV Mpro and chemical modification of the octapeptide". Peptides, 2004. 25(11): p. 1857-1864.
28. (Cited 94 times) Wei, D. and G. Patey, "Dynamics of molecular liquids: A comparison of different theories with application to wave vector dependent dielectric relaxation and ion solvation". The Journal of Chemical Physics, 93(2): p. 1399-1411.
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37. (Cited 79 times) Xu, Q., Y. Xiong, H. Dai, K.M. Kumari, Q. Xu, H.-Y. Ou, and Wei D.Q., "PDC-SGB: Prediction of effective drug combinations using a stochastic gradient boosting algorithm". Journal of theoretical biology, 2017. 417: p. 1-7.
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39. (Cited 78 times) Ge, N.-N., Y.-K. Wei, G.-F. Ji, X.-R. Chen, F. Zhao, and Wei D.Q., "Initial decomposition of the condensed-phase β-HMX under shock waves: molecular dynamics simulations". The Journal of Physical Chemistry B, 2012. 116(46): p. 13696-13704.
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peptide vaccines from hrHPVs E6 proteins using immunoinformatics and computational systems biology approaches". PloS one, 2018. 13(5): p. e0196484.

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516. Gurudeeban Selvaraj, Satyavani Kaliamurthi, Yang-Kai Wei, Keren Gu, Dong-Qing Wei: Abstract: Comprehensive gene expression meta-analysis and integrated bioinformatic studies of shared signatures between AD and SQ in NSCLC. International Conference on "From Computational Biophysics to Systems Biology 2018 (CBSB2018)", Shenzhen, China, on May 20-23, 2018, Shenzhen, China; 05/2018.
517. Satyavani Kaliamurthi, Gurudeeban Selvaraj, Yang-Kai Wei, Keren Gu, Dong-Qing Wei: Abstract: Designing of CD8+ and CD4+ T- - cell epitope-based vaccine by targeting whole genome sequence of Asian subtype Human papilloma virus 5. International Conference on "From Computational Biophysics to Systems Biology 2018 (CBSB2018)", on May 20-23, 2018, Shenzhen, China; 05/2018
518. Shaoliang Peng, Xiaoyu Zhang, Yutong Lu, Xiangke Liao, Kai Lu, Canqun Yang, Jie Liu, Weiliang Zhu, Dong-Qing Wei: mAMBER: A CPU/MIC collaborated parallel framework for AMBER on Tianhe-2 supercomputer. 2016 IEEE International Conference on Bioinformatics and Biomedicine (BIBM); 12/2016, DOI:10.1109/BIBM.2016.7822595
519. Fenglei Yang, Sijung Hu, Xiaoyun Ma, Harnani Hassan, Dong-Qing Wei: A new engineering approach to reveal correlation of physiological change and spontaneous expression from video images. BiOS SPIE 2015, San Francisco; 02/2015, DOI:10.1117/12.2077120
520. Peng Lian, Hao-Bo Guo, Jeremy C. Smith, Hong Guo, Dong-Qing Wei: The Catalytic Mechanism and Hyperthermophilic Nature of Cellulase TmCel12A Reveal a Possible Pathway to Improve the Efficiency of Cellulosic Biofuel Production. International Conference on Computational and Systems Biology; 01/2012
521. Peng Lian, Jue Li, Dongqi Wang, Dong-Qing Wei: ab initio Dynamics Simulations Reveal the Mechanism of Compound I's Formation during Catalytic Circle of Cytochrome P450cam. 3rd International Conference on Computational and Systems Biology; 10/2011
522. Peng Lian, Jing-Fang Wang, Dong-Qing Wei: Molecular Dynamics Studies on phospholamban in membranes. International Conference on Computational and Systems Biology; 10/2009
523. Peng Lian, Yongxiang Shi, Yuxiang Bu, Dong-Qing Wei: Study on Interaction between DNA and POU Cooperating with HMG by Molecular Dynamics Simulation. Theory and Applications of Computational Chemistry 2008, Shanghai, China; 09/2008
524. Jing-Yi Yan, Jing-Fang Wang, Dong-Qing Wei: Interactions of CYP2C9 with Different Substrates and its Implications for Metabolic Mechanism. Bioinformatics and Biomedical Engineering, 2008. ICBBE 2008. The 2nd International Conference on; 06/2008, DOI:10.1109/ICBBE.2008.45
525. Jing-Fang Wang, Lin-Li, Dong-Qing Wei: Discovery of Anti-Hiv Drugs Using Computer Aided Drug Designing Tools. Bioinformatics and Biomedical Engineering, 2007. ICBBE 2007. The 1st International Conference on; 08/2007, DOI:10.1109/ICBBE.2007.87

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526. Tangzhen Zhao, Yukun Wang, Qin Xu and Dong-Qing Wei, "Molecular Dynamics Simulations of Calcium Binding Sites in the RCK Domain of the Mthk Gating Ring", 59th Annual Meeting of the Biophysical-Society, Baltimore, MD, 2015.

527. Dong-Qing Wei, “Structural Bioinformatics and Chinese Traditional Medicine Database For Drug Design and Personalized Medicine”, J Antivir Antiretrovir 3 (4), 169 (ISSN: 1948 -5964).
528. D.R. Salahub, H. Guo, E. Proynov, S. Sirois, J.F. Truchon, and Dong-Qing Wei, “Biomolecular modeling with density functional theory and other tools: Aspects of enzymic mechanisms”, Book of Abstracts, 215th ACS National Meeting, Dallas, March 29-April 2 (1998), PHYS-264. Publisher: American Chemical Society, Washington, D. C.
529. Dong-Qing Wei and D.R. Salahub, “DFT ab initio molecular dynamics (MD) and combined DFT and MD simulation”, Book of Abstracts, 214th ACS National Meeting, Las Vegas, NV, September 7-11(1997), COMP-170. Publisher: American Chemical Society, Washington, D. C.
530. Dong-Qing Wei and Dennis R Salahub, “Density Functional Theory Ab Initio Molecular Dynamics and Combined Density Functional Theory and Molecular Dynamics Simulations”, ACS Symposium Series. 712, 159-171(1998). Publisher: American Chemical Society, Washington, D. C.
531. DR Salahub, F. Bohr, ME Casida, JG Guan, C. Jamorski and Dong-Qing Wei,” Electronic Response Properties From Density Functional Theory”, Book of Abstracts. 208, COMP-33 (1994).Publisher: American Chemical Society, Washington, D. C.

Presentations made at conferences (163)

1. Dong-Qing Wei, “Artificial Intelligence Supercomputing Precision Drug Discovery: Anti-Aging, Cancer Immunology and COVID-19”, 8th National Conference of Bioinformatics and Computational Biology, July 22-25, 2022, Guangzhou, China.
2. Dong-Qing Wei, “Artificial Intelligence Supercomputing Precision Drug Discovery: Anti-Aging and COVID-19”, China Big Data Technology Conference, Jan 23-24, 2021. A nationwide conference by the Chinese Computer Society at Changsha, Hunan.
3. Dong-Qing Wei, “Artificial Intelligence Supercomputing Precision Drug Discovery: Anti-Aging and COVID-19”, Symposium on New Technologies in Bioinformatics and AI, March 19-21, 2021, A nationwide conference by Xiangtan University at Xiangtan, Hunan.
4. Dong-Qing Wei, “Artificial Intelligence Supercomputing Precision Drug Discovery: Anti-Aging and COVID-19”, China Biomedical Technology Innovation and Development Summit Forum and the Second Xiangjiang Academician Forum Activity, May 08, 2021, A nationwide conference by Changsha Science and Technology Association, and Changsha High-tech Industrial Development Zone Management Committee at Xiangtan, Hunan.
5. Dong-Qing Wei, “Artificial Intelligence Supercomputing Precision Drug Discovery: Anti-Aging and COVID-19”, High-Performance Computing and Artificial Intelligence Technology Symposium, June 17, 2021, A nationwide conference organized by ACM SIGHPC CHINA, School of Information Science and Engineering, Hunan University, National Supercomputing Changsha Center at Changsha, Hunan.
6. Dong-Qing Wei, “AIDD and drug candidates by super-computing”, "Biorefining and Synthetic Biology" China-Thailand Cooperation and Exchange Forum, September 27, 2021, A bilateral conference organized by Shanghai Jiao Tong University, Thailand National Research Center for Genetic Engineering and Biotechnology (BIOTEC) at Shanghai.
7. Dong-Qing Wei, “AIDD and drug candidates by super-computing”, The 16th International Congress of Genomics, October 25-31, 2021, A global conference organized by BGI, The China National GeneBank (CNGB), GigaScience at Qingdao.

8. Dong-Qing Wei, “Artificial Intelligence Supercomputing Precision Drug Discovery: Anti-Aging and COVID-19”, The 10th National Conference on Bioinformatics and Systems Biology, A global conference organized by the Chinese Society of Bioinformatics at Chengdu.
9. Dong-Qing Wei, “Artificial intelligence supercomputing precision drug discovery: anti-aging and new crown”, The 14th Annual Conference of the Chinese Society of Biological Engineering, October 16-17, 2021, A nationwide conference organized by the Biological Resources Committee of Chinese Society of Biological Engineering, Shanxi Biological Engineering Society at Shanxi Jinzhong.
10. Dong-Qing Wei, “Artificial Intelligence Supercomputing Precision Drug Discovery: Anti-Aging and COVID-19”, 2021 3rd China Active Health Conference, October 22-24, 2021, A nationwide conference organized by China Active Health Innovation Alliance, Beijing Precision Medicine Society at Shanghai.
11. Dong-Qing Wei, “Artificial Intelligence Supercomputing Precision Drug Discovery: Anti-Aging and COVID-19”, ISBRA 2021 & ICBDS 2021, November 26-28, 2021, A nationwide conference by Shenzhen Institute of Advanced Technology, Chinese Academy of Sciences at Shenzhen.
12. Dong-Qing Wei, “Precision medicine and health research of lyrebellin”, Academician expert Jinan trip, November 02, 2021, organized by China Association for Science and Technology, Chinese Society of Biological Engineering at Jinan, Shandong.
13. Dong-Qing Wei, “AIDD and drug candidates by super-computing”, the fourth conference on Computational and Mathematical Bioinformatics and Biophysics, December 13-17, 2021, A bilateral conference organized by TSIMF Sanya, Hainan.
14. Dong-Qing Wei, “Artificial Intelligence Supercomputing Precision Drug Discovery: Anti-Aging and COVID-19”, The 11th Jiangsu Provincial Conference on Bioinformatics, December 04-05, 2021, A nationwide conference by Bioinformatics Professional Committee of Jiangsu Biomedical Engineering Society at Nanking.
15. Dong-Qing Wei, “Artificial Intelligence Supercomputing Precision Drug Discovery: Anti-Aging and COVID-19”, Wu Wenjun Artificial Intelligence Science and Technology Award 10th Anniversary Award Ceremony and 2020 Chinese Intelligent Industry Annual Conference, April 10-12 2021, A nationwide conference by the Chinese Society of Intelligent Engineering at Suzhou.
16. Dong-Qing Wei, “2020 China Big Data Technology Conference”, Attended Invited breakout sessions at the national conference organized by the Chinese Computer Society from January 23-24th, 2021 at Changsha, Hunan.
17. Dong-Qing Wei, “A nationwide Symposium on New Technologies in Bioinformatics and AI”, Attended the Report of the General Assembly organized by Xiangtan University from March 19-21, 2021 at Xiangtan, Hunan.
18. Dong-Qing Wei, “The 18th nationwide Yangtze River Delta Science and Technology Forum”, Invited reports organized by the Shanghai Association of Science and Technology, Jiangsu Science and Technology Association, Zhejiang Science and Technology Association, Anhui Science and Technology Association, Songjiang District People's Government on May 20th, 2021 at Shanghai.
19. Dong-Qing Wei, “A nationwide China Biomedical Technology Innovation and Development Summit Forum and the Second Xiangjiang Academician Forum Activity”, Reports of the

general assembly organized by Changsha Science and Technology Association, Changsha High-tech Industrial Development Zone Management Committee, Changsha Biomedicine (Gene Technology) Industry Chain Promotion Office, Hunan Pharmaceutical Industry Association on May 08, 2021, at Changsha, Hunan.

20. Dong-Qing Wei, “A nationwide 2021 High-Performance Computing and Artificial Intelligence Technology Symposium” organized by ACM SIGHPC CHINA, School of Information Science and Engineering, Hunan University, National Supercomputing Changsha Center on June 17, 2021, at Changsha, Hunan.
21. Dong-Qing Wei, “A nationwide 8th "From Atoms to Earth" – Symposium on High-Pressure Science and Earth Science”, organized by Key Laboratory of High Temperature and Pressure of Earth's Internal Matter, Chinese Academy of Sciences, Institute of Geochemistry, Chinese Academy of Sciences, Experimental Mineral, Petrological, and Geochemistry Professional Committee of Chinese Society of Mineralogy, Petrology, and Geochemistry, Fluid Geoscience Committee of Chinese Geophysical Society, High-Pressure Physics Committee of Chinese Physical Society, Chinese Interdisciplinary Science Society from July 2-5, 2021 at Guizhou, China.
22. Dong-Qing Wei, “A nationwide invited Symposium on Protein Structure Prediction Based on Next-Generation Supercomputing Platform”, organized by National Supercomputing Shenzhen Center from Wu Wenjun Artificial Intelligence Science and Technology Award 10thAnniversAugust 28-29, 2021 at Shenzhen.
23. Dong-Qing Wei, “A bilateral Biorefining and Synthetic Biology" China-Thailand Cooperation and Exchange Forum”, organized by Shanghai Jiao Tong University, Thailand National Research Center for Genetic Engineering and Biotechnology (BIOTEC) on September 27th, 2021 at Shanghai, China.
24. Dong-Qing Wei, “A nationwide Medical Mathematics Satellite Academic Conference”, participation organized by the Medical Mathematics Committee of the Chinese Mathematical Society on October 24th, 2021 at Kunming, Yunnan.
25. Dong-Qing Wei, “The nationwide 10th National Conference on Bioinformatics and Systems Biology”, Invited breakout sessions organized by the Chinese Society of Bioinformatics from October 25-28, 2021 at Chengdu.
26. Dong-Qing Wei, “The 14th nationwide Annual Conference of the Chinese Society of Biological Engineering” organized by Biological Resources Committee of Chinese Society of Biological Engineering, Shanxi Biological Engineering Society from October 16-17, 2021 at Shanshi, Jinzhing.
27. Dong-Qing Wei, “The nationwide 2021 3rd China Active Health Conference”, organized by China Active Health Innovation Alliance, Beijing Precision Medicine Society from October 22-24, 2021 at Shanghai.
28. Dong-Qing Wei, “The 9th nationwide China Computer Society Big Data Academic Conference”, participation organized by the Chinese Computer Society from November 19-21, 2021 at Guangzhou, Guangdong.
29. Dong-Qing Wei, “ISBRA 2021 & ICBDS 2021”, A nationwide Report of the General Assembly organized by Shenzhen Institute of Advanced Technology, Chinese Academy of Sciences from November 26-28, 2021 at Shenzhen, China.

30. Dong-Qing Wei, “Academician expert Jinan trip”, A nationwide trip for a report of the general assembly organized by China Association for Science and Technology, Chinese Society of Biological Engineering on November 2nd, 2021 at Jinan, Shandong.
31. Dong-Qing Wei, “The fourth nationwide conference on Computational and Mathematical Bioinformatics and Biophysics”, organized by TSIMF from December 13-17, 2021 at Sanya, Hainan.
32. Dong-Qing Wei, “The 11th nationwide Jiangsu Provincial Conference on Bioinformatics”, organized by Bioinformatics Professional Committee of Jiangsu Biomedical Engineering Society from December 04-05, 2021 at Nanking.
33. Dong-Qing Wei, “A nationwide Wu Wenjun Artificial Intelligence Science and Technology Award 10th Anniversary Award Ceremony and 2020 Chinese Intelligent Industry Annual Conference”, attended invited breakout sessions organized by the Chinese Society of Intelligent Engineering from April 10-12th 2021 at Suzhou.
34. Dong-Qing Wei, “Artificial Intelligence Supercomputing and Accurate Drug Discovery”, Supercomputing and AI-assisted COVID-19 Prevention and Cure, Dec. 6-8, 2020, The 3rd Conference of Computational Biology and Bioinformation Processing, Yantai, China, plenary talk.
35. Dong-Qing Wei, “Artificial Intelligence Supercomputing and Accurate Drug Discovery”, Supercomputing and AI-assisted COVID-19 Prevention and Cure, Aug. 28, 2020, Online Conference, invited talk.
36. Dong-Qing Wei, “Artificial Intelligence Supercomputing and Accurate Drug Discovery”, The 3rd Worldwide Chinese Conference of Computational Biology, Aug. 3-6, 2020, Online Conference, invited talk.
37. Dong-Qing Wei, “Artificial Intelligence Supercomputing and Accurate Drug Discovery”, Big Data and AI, On-line Conference, March 13-16, 2020, invited talk.
38. Dong-Qing Wei, “Thermal Decomposition of The Solid Phase Nitromethane: Ab Initio Molecular Dynamics Simulations”, Workshop of Shock Wave Physics, Aug. 19-23, Shanghai, China, plenary talk.
39. Dong-Qing Wei, G.N. Patey, "Rotational Motion in Molecular Liquids", "The Canadian Society for Chemistry Conference", June 1989, Victoria, B.C.
40. Dong-Qing Wei, G.M. Torrie and G.N. Patey, "Molecular Solvent Model For an Electrical Double Layer: Effects of Ionic Polarizability", "76th Canadian Society for Chemistry Conference and Exhibition", June 1993, Sherbrooke, Quebec, Canada.
41. Dong-Qing Wei and Abbas Khan, “Identification of Novel Drug Targets for Diamond Black-fan Anemia (DBA) Based on RPS19 Gene Mutation, Using Protein-Protein Interaction Network”, Invited Talk, 2017 International Conference of System Biology, Shenzhen, China, Aug. 18-21, 2017.
42. Jing-Yi Yan, Dong-Qing Wei, Jing-Fang Wang, “Interactions of CYP2C9 with Different Substrates and its Implications for Metabolic Mechanism”, The 2nd IEEE International Conference on Bioinformatics and Biomedical Engineering, Wuhan, May 2008 (Co-chairman and invited talk).
43. Jing-fang Wang, Lin Li, Dong-Qing Wei and Kuo-Chen Chou, “Discovery of Anti-HIV Drugs Using Computer Aided Drug Design Tool”, The 1st IEEE International Conference on

Bioinformatics and Biomedical Engineering, Wuhan, July 2007(Division chairman and invited talk).

44. Dong-Qing Wei, “Ultra-fast Chemical Reactions and Energetic Materials Under Shock Wave”, Symposium on High Pressure Science and Earth Science, Xiangyang, China, Aug. 2-4, 2019.
45. Dong-Qing Wei, “Personalized Medicine in Era of Bio Data-Discovery of WGX-50 and Anti-aging Function”, Huaxiang International Forum, Changsha, China, June 16-18, 2019.
46. Dong-Qing, Wei, “Rare Event Dynamics Involving Membrane Systems and CADD”, 2019 Symposium of Jiangsu and Zhejiang Bioinformatics, Wuxi, China, April 19, 2019.
47. Dong-Qing Wei, “Precision Drug Discovery Based on Plant Extractions and Chinese Traditional Medicine Database”, 6th National Conference on Computational Biology and Bioinformatics, Chengdu, China, March 29-31, 2019.
48. Dong-Qing Wei, “Deep Learning For Precision Medicine of Cancer Treatments”, 8th National Conference on System Biology and Bioinformatics, Macau, Oct. 22-24, 2018.
49. Qin Xu and Dong-Qing Wei, “Multiple interconverting conformations of C99 dimer characterized by MD simulations”, International Workshop on Molecular Simulation 2018, Shanghai, China, August 25 - 27, 2018.
50. Dong-Qing Wei, “Discovery of Wgx-50 and its Anti-Aging Function”, Keynote Talk, 17th, Chinese National Conference of Interdisciplinary Sciences, Hulunbeier, China, Aug. 01-05, 2018.
51. Ru-Gu and Dong-Qing Wei, “Rare Event Dynamics Involving Membrane Systems and CADD”, Plenary Talk, 2nd Chinese Conference on Computational Biophysics and Molecular Simulations, Zhuhai, China, June 07-10, 2018.
52. Dong-Qing Wei, “Wgx-50 and its Role Anti-Aging and Radiation”, Plenary Talk, 1st High Level Forum of Radiation Biology, Ningbo, China, June 06-08, 2018.
53. Dong-Qing Wei, “Discovery of Wgx-50 and its Anti-Aging Function”, Keynote Talk, 11th Chinese National Neurology Doctors, Changsha, China, June 01-04, 2018.
54. Dong-Qing Wei, “Rare Event Dynamics Involving Membrane Systems and CADD”, Invited Talk, Computational Biophysics and Systems Biology” (CBSB2018), Shenzhen, China, May 20-23, 2018.
55. Qin Xu and Dong-Qing Wei, “Rare Event Dynamics Involving Membrane Systems and CADD”, Invited Talk, 5th National Bioinformatics Conference organized by Chinese Bio-Engineering Society, Tangshan, China, April 21-22, 2018.
56. Dong-Qing Wei, “WGX-50 and its Role As a Drug Candidate of AD and Anti-Aging”, Plenary Talk, Symposium On Natural Medicine, Hangzhou, China, Aug. 9-12, 2017.
57. Dong-Qing Wei, “Personalized Drug, Precision Medicine, WGX-50 and its Role As a Drug Candidate of AD and Anti-Aging”, Plenary Talk, Conference on Functional Genomics and System Biology, Harbin, China, August 9-11, 2017.
58. Dong-Qing Wei, “SNPs of CYP450 and Personalized Drug, Precision Medicine”, Plenary Talk, 3rd Conference on Digital Medicine and Big Data Analysis, Changchun, China, August 6-8, 2017.
59. Dong-Qing Wei, “Chemistry and Phase Transition of Deep Carbon”, Plenary Talk, 7th Conference From Atom to Earth, High Pressure Earth Science, Changchun, China, August 6-8, 2017.

60. Dong-Qing Wei and Guang-Fu Ji, “Phase Transition and The Ultra-fast Chemical Reactions of Energetic Materials Explored by Ab Initio MD Simulations”, Plenary Talk at the 10th Conference of Computational Nano-Science and New Materials, Jishou, China July 16-19, 2017.
61. Dong-Qing Wei and Guang-Fu Ji, “Ultra-fast Chemical Reactions of Energetic Materials Explored by Ab Initio MD Simulations”, Invited Talk at the 13th National Conference of Quantum Chemistry, Dalian, China June 8-11, 2017.
62. Dong-Qing Wei, “Initial Chemical Reactions of Explosives Under Shockwave Impact”, the deMon Workshop, Calgary, Canada, May 11-17, 2017.
63. Dong-Qing Wei, “SNPs of CYP450, Personalized Drug, Precision Medicine, WGX-50 and its Role As a Drug Candidate of AD and Anti-Aging”, Plenary Talk at the 4thNational Conference of Bioinformatics, organized by the Bioinformatics Division, Chinese Biotechnology Association, Changsha, China, April 22-24, 2017.
64. Dong-Qing Wei, “Application and Assessment of Health Medicine Big Data”, Plenary Talk at the First National Conference on the Assessment and Protection of Health &Medicine Big Data Application, organized by the Division of the Assessment and Protection of Health &Medicine Big Data Application, Chinese Association of Health Information, Beijing, China, April 7-8, 2017.
65. Dong-Qing Wei, “SNPs of CYP450, Personalized Drug, Precision Medicine, WGX-50 and its Role As a Drug Candidate of AD and Anti-Aging”, Plenary Talk at the 2016 Big Dada Technology Conference, Beijing, China, Dec. 8-10, 2016.
66. Dong-Qing Wei, “Rare Event Dynamics and Free Energy of Membrane Systems”, Invited Talk at the 4th International Conference on Molecular Simulation (ICMS-2016), Shanghai, China, October 23-26,2016.
67. Dong-Qing Wei, “Rare Event Dynamics, Ion Permeation and Free Energy of Membrane Systems”, Invited Talk at the 7th National Conference of Bioinformatics and System Biology, Chengdu, China, October 7-9,2016.
68. Dong-Qing Wei, “Simulations of Protein Dynamics on Super-Computer and CADD”, Symposium of High-Performance Computation, Beijing, September 22-24, 2016.
69. Dong-Qing Wei, “Rare Event Dynamics of Ion Permeation Across Membranes and Chains”, Theory and Application of Computational Chemistry, Seattle, USA, August 13-September 5, 2016.
70. Dong-Qing Wei, “An Improved Feature-Based Approach to Predict Effective Drug Combinations”, Invited Talk at the 10th International Conference on Systems Biology, Weihai, China, August 19-22, 2016.
71. Dong-Qing Wei, “Precision Medicine Informatics”, Plenary Talk at the 16th National Conference of Interdisciplinary Sciences, Dandong, China, August 5-8, 2016.
72. Dong-Qing Wei, “SNPs of CYP450 and Molecular Metabolism”, Plenary Talk at the 7th National Conference of Microbial Genetics, Hohhot, China, August 5-8, 2016.
73. Dong-Qing Wei, “SNPs of CYP450and Molecular Metabolism and Toxicity”, Plenary Talk at the6th Agricultural Microbiology, 15th Insecticidal Microorganism, 11th entomogenous fungi, Shanghai, China, July 17-19, 2016.
74. Dong-Qing Wei, “Free Energy Calculations of Membrane Systems and CADD”, 2016 Shanghai Workshop on Frontiers in Molecular Biophysics, Shanghai, China, July 23-26, 2016.

75. Dong-Qing, Wei, “QM/MM Studies of Enzyme Catalysis”, Plenary Talk at The 21st International Workshop on Quantum Systems in Chemistry, Physics, and Biology (QSCP-XXI) Vancouver, Canada, July 2-9, 2016.
76. Dong-Qing Wei, “SNPs of CYP450and Molecular Metabolism and Toxicity”, Plenary Talk at the 2016 Cross-Strait Predictive Toxicology Conference:Environment, Food and Health, Taichung, Taiwan, May 5-7, 2016.
77. Dong-Qing Wei, “Ab Initio MD and Fast Reactions of Energetic Materials”, Plenary Talk at the International Workshop Molecular Simulation, 2016, Xian, China, April 15-17, 016.
78. Dong-Qing Wei, “HPC, Personalized Medicine and WGX-50”, Plenary Talk at the Conference of Big Data and Precision Medicine, Shanghai, China, March 25-27, 2016.
79. Dong-Qing Wei, “Dynamics of Passive Membrane Permeations”, Plenary Talk at the High-Performance Computing Symposium, Changshu, Jiangsu, China, Nov. 27-28,2015.
80. Dong-Qing Wei, “High Pressure Physics and Chemistry of Some Carbon Containing System in The Geophysical Environment”, Plenary Talk at the 5th National Conference on High Pressure Geophysics-From Atoms to Earth, Beijing, China, Nov. 28-30, 2015.
81. Dong-Qing Wei, “Drug Screening Technology Based on The Traditional Chinese Medicine Database and Anti-Aging Function of Wgx-50, a Molecule Extracted From Sichuan Pepper” Plenary Talk at the Annual National Conference on Active Components From Herbs, Changsha, China, Nov. 11-18, 2015.
82. Yukun Wang, Ruoxu Gu and Dong-Qing Wei, “Free Energy Calculation For Membrane Systems and CADD”, Invited Talk at the 9th International Conference on Systems Biology (ISB 2015), Aug. 21-24, 2015, Luoyang, China.
83. Yukun Wang, Ruoxu Gu and Dong-Qing Wei, “Free Energy Calculation For Membrane Systems and CADD”, Invited Talk at the 13th National Conference on Computational Chemistry, Nov. 19-22, 2015, Guangzhou, China.
84. Dong-Qing Wei, “Drug Screening Technology Based on The Traditional Chinese Medicine Database and Anti-Aging Function of Wgx-50, a Molecule Extracted From Sichuan Pepper”, Plenary Talk at the 2nd National Conference on New and Green Technology of Pharmacology, Lasha, China, July 25-27, 2015.
85. Yukun Wang, Ruoxu Gu and Dong-Qing Wei, “Free Energy Calculation For Membrane Systems and CADD”, Plenary Talk at the Annual National Conference on System Biology and Bioinformatics, Zhuhai, China, May 5-7, 2015.
86. Dong-Qing Wei, Yukun Wang, Ruoxu Gu, Huameng Fan, Dan Hu and Jacob Ulmschneide, “Rare Event Dynamics: Ion Transportation Through Protein channels and Across Membranes and CADD”, Plenary Talk at the Young Scholar Frontier Symposium on Quantitative Biology Development, Beijing, China, May 8-10, 2015.
87. Dong-Qing Wei, “Physics and Chemistry of Deep Carbon Circulation”, Plenary Talk at the 3rd National Conferences on Geo-biochemistry, Wuhan, China, March 17-18, 2015.
88. Dong-Qing Wei, “A Drug Candidate from Traditional Chinese Medicine and Its Potential Role Against AD And in Anti-aging”, Symposium of Traditional Medicine, Cha University and Cha Hospitals, Seoul, Korea, Jan. 19-22, 2015.
89. Dong-Qing Wei, Yukun Wang, Ruoxu Gu, Huameng Fan, Dan Hu and Jacob Ulmschneide, “Rare Event Dynamics: Ion Transportation Through Protein channels and Across Membranes

and CADD", Plenary Talk at the Workshop on Frontiers of Molecular Simulations, Beijing, China, Jan. 4-5, 2015.

90. Yukun Wang, Ruoxu Gu and Dong-Qing Wei, "Free Energy Calculation For Membrane Systems and CADD", Invited Talk at 6th National Conference on Bioinformatics and System Biology, Nanjing, China, Oct. 6-9, 2014.
91. Dong-Qing Wei, Kai Xu, Yanzhi Bai, Shouxin Cui and Guangfu Ji, "Preliminary Studies of Carbon Circulation- Chemical Reactions of Systems Consists of C, H, N, O in The High-Pressure Regime, And Solid Phases of Carbon Dioxide", Plenary talk at The Oriental Forum, Shanghai, China, Sept. 28-30, 2014.
92. Yukun Wang, Ruoxu Gu and Dong-Qing Wei, "Rare Event Dynamics: Ion Transportation Through Protein channels and Across Membranes and CADD", Plenary Talk at 14thNational Conference of Interdisciplinary Sciences, Zhengzhou, China, Sept. Aug. 7-10, 2014.
93. Nina Ge, Guangfu Ji and Dong-Qing Wei, "Quantum Chemical Simulation of Chemical Reactions in the decomposition of explosives", Plenary Talk at the 10th National Explosion Mechanics, Guiyang, July 26-30, 2014.
94. Yukun Wang, Ruoxu Gu and Dong-Qing Wei, "Rare Event Dynamics: Ion Transportation Through Protein channels and Across Membranes and CADD", Plenary Talk at 26th Canadian Symposium on Theoretical and Computational Chemistry (CSTCC), Montreal, Quebec, Canada, July 1-5, 2014.
95. Peng Lian, Dong-Qing Wei, Hong Guo, Jeremy Smith "QM/MM Studies of Enzyme Catalysis", Plenary Talk at deMon workshop, Los Cabos, Mexico, April 28-May 1st, 2014.
96. Dong-Qing Wei and Yan-Zhi Bai, "Compression and Chemical Reactions For Systems Consists of C, H, N, O, And High Pressure Phases of Carbon Dioxide and Para-xylene (p-xylene)", 2nd Conference on Geochemistry and Geo-biochemistry", Wuhan, March 16-18, 2014.
97. Dong-Qing Wei, "Bioinformatics Studies of CYP450 and Personalized Drug Metabolism", Plenary Talk at the 4th International Conferences on Computational and System Biology (ICCSB), Shenzhen, China, Nov. 14-16, 2013.
98. Yukun Wang, Ruoxu Gu and Dong-Qing Wei, "Rare Event Dynamics: Ion Transportation Through Protein channels and Across Membranes", Invited talk at 12th National Computational Chemistry Conference, Suzhou, China, Oct. 21-24, 2013.
99. Ruoxu Gu, Yukun Wang and Dong-Qing Wei, "Rare Event Dynamics: Ion Transportation Through Protein channels and Across Membranes", Invited talk at 6th Asian and Pacific Conference on Theoretical and Computational Chemistry (APCTCC6), Gyeongju, Korea, July 10-13, 2013.
100. Li Li, Hai Dai and Dong-Qing Wei, "Bioinformatics Studies of CYP450 SNPs and Personalized Drug Metabolism", Invited talk at the 94th AAAS Pacific Division Annual Meeting, Las Vegas, USA, June 16-19, 2013.
101. Kai Xu, Juqiang Jiang and Dong-Qing Wei, "Introduction to deMon-GUI and QM/MM Studies of Enzyme Catalytic Reactions", Plenary Talk at deMon workshop, Toulouse, France, June 20-24, 2013.
102. Dong-Qing Wei, Kai Xu, Yanzhi Bai, Shouxin Cui and Guangfu Ji, "Preliminary Studies of Carbon Circulation- Chemical Reactions of Systems Consists ofC, H, N, O in The High Pressure Regime, And Solid Phases of Carbon Dioxide", Plenary talk at Symposium ofHigh

Pressure Science and Technology in Memory of Prof. Fuqian Jing, Wuhan University of Science and Technology, Wuhan, China, Sept. 24-27, 2012.

103. Dong-Qing Wei, Yukun Wang, Ruoxu Gu, Huameng Fan, Dan Hu and Jacob Ulmschneider, "Rare Event Dynamics and Its Applications on the Free Energy Calculations for Membrane Protein Systems", Invited talk at the Theory and Application of Computational Chemistry (TACC 2012), Pavia, Italy, Sept. 1-8, 2012.
104. Dong-Qing Wei, "Simulations of Chemical and Biological Systems From Explosives to Membrane Proteins", Plenary talk at the Worldwide Chinese Computational Biology and Molecular Simulation Conference, Dalian, Aug. 9-12, 2012.
105. Dong-Qing Wei, Ruo-Xu Gu, Peng Lian and Huai-meng Fan, "Structural Bioinformatics and Chinese Traditional Medicine Database For Drug Design", Invited talk at the 5th National Conference of Bioinformatics, Harbin, Aug. 7-10, 2012.
106. Dong-Qing Wei, "Molecular Simulations of Solid Explosives", Plenary talk at the 9thNational Conference on Explosive Mechanics, Xining, China, July26-31 2012.
107. Dong-Qing Wei, "Computer Simulations A Must-having Tools for Biological and Material Sciences", Plenary talk at the 15thNational Conference of Chinese Interdisciplinary Sciences", Yinchuan, China, Aug. 1-4, 2012.
108. Dong-Qing Wei, Ruo-Xu Gu, Peng Lian and Huai-meng Fan, "Simulations of Chemical and Biological Systems From Explosives to Membrane Proteins", invited talk at the Professor Nick Quirke 60th birthday symposium at Imperial College of London, London, England, July 6, 2012.
109. Dong-Qing Wei, "Structural Bioinformatics and Chinese Traditional Medicine Database For Drug Design", invited talk at the International Symposium on Molecular Cognition and Translational Research of Neuropsychiatric Disorders, in Shanghai, China, April 28-30, 2012.
110. Dong-Qing Wei, "Structural Bioinformatics and Chinese Traditional Medicine Database For Drug Design", Invited talk at The 28th Congress of Chinese Chemical Society, Chengdu, China, April 13-16, 2011.
111. Dong-Qing Wei, "Structural Bioinformatics and Chinese Traditional Medicine Database For Drug Design and Personalized Medicine", invited talk at the International Conference and Exhibition on Virology, Boston, USA, 2011, 5-7 September 2011.
112. Dong-Qing Wei, "Reaction Mechanism of Solid Explosive", Invited talk at The National Conference on Theoretical and Quantum Chemistry, Hefei, China, July 2011.
113. Dong-Qing Wei, "Reaction Mechanism of Solid Explosive", Plenary talk at Conference From Atom to Earth, Dalian, China, July 2011.
114. Dong-Qing Wei, "Reaction Mechanism of Solid Explosive", Plenary talk at The National Conference on Dynamics Response, Tianyuan, China, July 2011.
115. Dong-Qing Wei, "Structural Bioinformatics, Traditional Chinese Medicine Database (TCMD) and Personalised Drug Design", Asian Biotechnology Congress, May 11-15, Shanghai, China, Invited talk.
116. Dong-QingWei, "Computational Chemistry for Some Real Chemical and Biological Problems", Plenary talk at deMon Workshop, Bremen, Germany, June 2011.
117. Dong-Qing Wei, "Computational Chemistry For Some Real Chem/Bio Problems: Reaction Mechanism of Explosives, Personalized Drug Design, Membrane Proteins and Protein-DNA Interactions", Indian Theoretical Chemistry Symposium, Dec. 8-12, Kanpur, India, plenary talk.

118. Dong-Qing Wei, “Structural Bioinformatics For Real Biological Problems: Personalized Drug Design, Membrane Proteins And The Protein-DNA Interactions”, Sino-German Workshop on Computational systems biology approaches for cancer research and biomarker discovery, January 11-15, 2010 Zhejiang University, Hangzhou, China, invited talk.
119. Dong-Qing Wei, “Structural Bioinformatics, Traditional Chinese Medicine Database (TCMD) and Personalized Drug Design”, 2008 Analysis of Effective Components of Chinese Traditional Medicines, Haikou, Nov. 11-13, 2009, plenary talk.
120. Dong-Qing Wei, “Structural Bioinformatics, Traditional Chinese Medicine Database (TCMD) and Personalized Drug Design”,2009 International Workshop on Computational and Integrative Biology, a satellite meeting of the International Conference of Integrative Biology, September 18th to 20th, 2009, Hangzhou, China, invited talk.
121. Dong-Qing Wei, “Structural Bioinformatics, Traditional Chinese Medicine Database (TCMD) and Personalized Drug Design”, Recent Progress in Computer Simulations in Molecular Sciences, Seoul, Korea, June 14-16, 2009, plenary talk.
122. Dong-Qing Wei, “Structural Bioinformatics, Traditional Chinese Medicine Database (TCMD) and Personalized Drug Design”, Westlake International Conference on Personalized Medicine, Hangzhou, China, May 29-30, 2009, invited talk.
123. Dong-Qing Wei, “Structural Bioinformatics, Traditional Chinese Medicine Database (TCMD) and Personalized Drug Design”, 2008 World Gene Congress, Fushan, Oct. 5-7 2008, invited talk.
124. Dong-Qing Wei, “Structural Bioinformatics, Traditional Chinese Medicine Database (TCMD) and Personalized Drug Design”, 2008 Analysis of Effective Components of Chinese Traditional Medicines, Shenzhen, Oct. 6-8, 2008, invited talk.
125. Dong-Qing Wei, “Structural Bioinformatics, Traditional Chinese Medicine Database (TCMD) and Personalized Drug Design”, Theory and Application of Computational Chemistry (TACC 2008), Shanghai, Sept. 23-27 2008, chairman and plenary talk.
126. Dong-Qing Wei, “Structural Bioinformatics, Traditional Chinese Medicine Database (TCMD) and Personalized Drug Design”, 3Rd National Conference on Bioinformatics and System Biology, Wuhan, Oct.7-9 2008, invited talk.
127. Dong-Qing Wei, “Structural Bioinformatics and Personalized Drug Design”, 5th MMPH Congress, Emeishan, Aug. 2008. Plenary talk and 5th Jiao Shanqing MMPH award.
128. Lin Li and Dong-Qing Wei, “Discovery of Drugs Using Computer Aided Drug Design Tool”, 10th International Congress on Amino Acids and Proteins, Chalkidiki, Greece, August 2007 (invited talk).
129. Jing-fang Wang and Dong-Qing Wei, “Molecular Modeling of CYP450 and Personalized Drug Design”, 9th Computational Conference of Chinese Chemical Society, Chengdu, Aug. 2007.
130. Dong-Qing Wei, “Computer Aided Drug Design Against HIV Based on Traditional Chinese Medicine Database”, World AIDS Day, Tianjin, Nov. 2006 (invited talk).
131.
132. Dong-Qing Wei, “Inhibitor Design Against Viruses”, International Symposium for Chinese Medicinal Chemists, ISCMC, Nanjing, October 2006(invited talk).
133. Dong-Qing Wei, “Bioinformatics and Inhibitor Design Against Viruses”, 25th Chinese Chemical Societies, Changchun, China, July 2006(invited talk).

134. Liu Hong, Zhao Jijun, WEI Dong-Qing, GONG Zizheng, First-Principles Study of Solid Nitromethane under High Pressure, International Autumn Seminar on Propellants, Explosives and Pyrotechnics, Beijing, Nov. 2005 (invited talk).
135. Weina Gao and Dong-Qing Wei, “Bioinformatics and Its Application on Inhibitor Design Against SARS”, 3rd International Symposium Computational Methods in Toxicology and Pharmacology Integrating Internet Resources (CMTPI-2005), Shanghai, Oct. 2005.
136. Dong-Qing Wei and Qishi Du, “A Combined Study of Ab Initio Quantum Mechanics and Integral Equation Theory in Three-Dimensions”, 9th Quantum Chemical Conference, Guilin, Oct. 2005(invited talk and session chair).
137. Qishi Du and Dong-Qing Wei et al invited talks of 8 papers on “Studies of the SARS drug design” and other research, Chinese Chemical Societies, Changsha, P.R. China, April 2004 (invited talk).
138. Dong-Qing Wei, invited talk, “Bioinformatics And Its Application to Drug Design Against SARS”, International Conference on Theory and Application of Computational Chemistry (TACC), Geonjiu, Korea, Feb. 2004(invited talk).
139. Dong-Qing Wei, plenary talk, “ab initio Molecular Dynamics Simulations of Molecular Liquids”, 12th High Pressure Physics Conference, Huangshan, P.R. China, Sept. 2004 (plenary talk).
140. Jijun Zhao, Hong Liu, Zi-Zheng Gong ad Dong-Qing Wei, invited talk, “Ab Initio Studies of Organic Molecular Crystals”,Xiamen, P.R. China, Nov. 2004(special invited talk).
141. Zi-Zheng Gong, Zhang Xu-Dong, Han Gao, He Bi, Hong Liu, Dong-Qing Wei and Guo Yongxin, invited talk “New Progress in Metallic Hydrogen Research”, Xiamen, P.R. China, Nov. 2004.
142. Rui Zhang, Yu Ji, Aixiu Li, Xin Zhang, Qishi Du, Kuo-Chen Chou, and Dong-Qing Wei, “Scoring and Docking Studies of the SARS-CoV Mpro binding with a few inhibitors”, The Second Annual World Congress, The Human Proteome Organization, Montreal, 2003 (invited talk).
143. S.S. Decker and T.K. Woo, Dong-Qing Wei and F. Zhang, “Combined QM/MM and Ab Initio Molecular Dynamics of Nitromethane at High Pressure”, in “12th International Detonation Symposium”, San Diego, 2002.
144. Dong-Qing Wei, F. Zhang and T. K. Woo, “First-Principle Simulations of Energetic Molecular Liquids”, in “Shock Wave Physics”, Atlanta, 2001.
145. Dong-Qing Wei, "Application of Quantum/Classical Molecular Dynamics to Biologically Interesting Systems", in "New Perspectives for Computer-aided Drug Design", Montreal, April 1999.
146. Dennis R. Salahub, Hong Guo, Emil Proynov, Suzanne Sirois, Jean-Francois Truchon and Dong-Qing Wei, "Biomolecular Modeling with Density Functional Theory and Other Tools: Aspects of Enzymatic Mechanisms", in "ACS Meeting", Dallas, 1998 (invited talk).
147. Dennis R. Salahub, Steeve Chrétien, Anne Milet, Emil Proynov, Suzanne Sirois, Dong-Qing Wei, "Activation Energies and Dynamics from DFT: How Good Are the Functionals?" in "DFT Based Descriptors of Reactivity: Concepts And Applications", Cracow, Dec. 3-5, 1998 (invited talk).

148. Dong-Qing Wei "Recent Advances on the Molecular Theories of Electrolyte Solutions: Equilibrium Structures, Thermodynamics and Dynamics", “The Problems of Solvation and Complex Formation in Solutions”, Ivanovo, Russia, 1998 (plenary talk).
149. Dong-Qing Wei, "Ab Initio MD and Its Application", “The Second International Conference on Frontiers of Physics” and “Joint Meeting of Chinese Physical Societies”, on the Occasion of Professor Dayou Wu's 90th birthday, Taipei, 1997.
150. Dong-Qing Wei and D.R. Salahub, "DFT Ab Initio Molecular Dynamics and Combined DFT and Molecular Dynamics Simulations", “214th American Chemical Society National Meeting”, Las Vegas, September, 1997.
151. Dong-Qing Wei and D.R. Salahub, "Hydrated Proton Clusters: Structure, Spectroscopy and Ab Initio Dynamics", “Gordon Research Conference”, NH, USA,Aug 1996.
152. Dong-Qing Wei "Theory and Simulation of Strongly Interacting Dipolar Fluids: Ferroelectric Liquid Crystals, Ferrofluids and Electrorheological Fluids", “The First International Conference on Frontiers of Physics: Looking to the 21st Century”, Shantou, 1995.
153. D. Salahub, Dong-Qing Wei, M. Leboeuf, Hong Guo, V. Malkin, O. Olga, T. Woolf and B. Roux, "Chemical Reactivity in Complex Environments Studies With Density Functional Theory and Other Tools", oral presentation in the Scientific Session, Network of Centres of Excellence in Molecular and Interfacial Dynamics, Victoria, B.C., May4-7, 1994.
154. Dong-Qing Wei, A. Chandra and G. Patey, "Ion Solvation Dynamics", “The Second Canadian Computational Chemistry Conference”, Kingston, May 21-25, 1994.
155. Dong-Qing Wei and G.N. Patey,"Ferroelectric Liquid Crystals: a Computer Simulation Study", 34th IUPAC Congress, Beijing, August 1993, “76th Canadian Society for Chemistry Conference and Exhibition”, June, 11, Sherbrooke, Quebec, Canada, the Scientific Session, 1992, Network of Centers of Excellence in Molecular and Interfacial Dynamics, Vancouver, B.C., Canada.
156. Dong-Qing Wei and G.N. Patey, "Dynamics in a Ferroelectric Nematic Phase", "The Gorden Conference on Water and Aqueous Solution", August 1992, New London, NH, USA.
157. Chandra, Dong-Qing Wei and G.N. Patey, "Dielectric Relaxation of Electrolyte Solutions", “The Gorden Conference on Water and Aqueous Solution", August 1992, New London, NH, USA.
158. Dong-Qing Wei and G.N. Patey, "The Double Layer Structure in a Model Electrolyte Solution of Polarizable Anion", "The Gorden Conference on Water and Aqueous Solution", August, 1992, New London, NH, USA.
159. Dong-Qing Wei, G.N. Patey, "Dielectric Relaxation of Molecular Liquids", “The Gorden Conference on Water and Aqueous Solution", August 1990, New London, NH, USA.
160. Dong-Qing Wei, J.J. Zhu, J.S. Lu and L. Blum, "Thermodynamic Behavior of Salt in Mixed Solvents", The Gorden Conference on Water and Aqueous Solution”, August 1986, New London, NH, USA.
161. Dong-Qing Wei and J.S. Lu, "The Salt Effect on the Gas-liquid Equilibrium in Mixed Solvents", “The Second National Conference on Thermodynamics, Thermochemistry and Thermoanalysis”, September 1984, Wuhan, China.
162. Dong-Qing Wei, "Time Oscillation Study of a Two Molecule Three Intermediate Reaction", “The Fourth National Conference on Non-equilibrium Statistical Mechanics", October 1984, Guilin, China.

163. Dong-Qing Wei, "Markov Processes in Meteorology", “Symposium on the Application of Statistical Physics on Meteorology", September 1983, Xinjiang, China.

Membership and Professional Affiliations

Fellow, The Royal Society of Chemistry, since 2022;

Editor-in-Chief, “Interdisciplinary Sciences - Computational Life Sciences”, snice 2009

Editor-in-Chief, “Current Computer Aided Drug Design” , snice 2022;

Co-Editor (Bioinformatics), “Current Chinese Sciences” , since 2020;

Editorial Advisor:The Royal Society of Chemistry book series on Theoretical & Computational Chemistry.;

Editorial Board: “Molecular Simulation”, “Journal of Molecular Modeling and Graphics”, “Scientific Reports”, “Biomolecules”, “Protein & Peptide Letters”, “Journal of Atomic and Molecular Physics (In Chinese: “Chinese Journal of High Pressure Physics”, “J. Biomedical Research”).

Referees of the following journals

Phys. Rev. Letters, Phys. Reviews, JACS, Bioinformatics, Briefing in Bioinformatics, J. Chem. Inf. Model., JCTC, J. Med. Chem., Biophys. J., J. Biophys., BMC Systems Biology, J. Theor. Bio., Scientific Report, Current Med. Chem., Med. Chem., J. Chem. Phys. Chem. Phys. Lett., J. Phys. Chem., PCCP, J. Comp. Chem., Chem. Phys., BBRC, Mol. Phys., Mol. Simulation, BMC Microbiol., BBA, Amino Acids, Int. J Bio Macromol, Int. J. Infectious Diseases, Biotech. Prog., IEEE Trans. Comp. Bio. and Bioinformatics, App. Biochem. and Biotech., Cancer Lett., Bioorg. Med. Chem., Protein Peptide Lett., Pharmacogenetics, J. Mol. Graph and Modeling, Acta Chem. Sin., Chinese Physics Letter, J. Energetic Materials, Chem. J. of Chinese Universities, Chinese Science Bull., Comp. Phys., PloS One, PLoS Comp Bio., Nature Communication, App Phys., App Phys. Lett., Mol. Liquids.

Chairman, International Association of Scientists in the Interdisciplinary Areas (IASIA);

Vice Chairman, International Society of Bioinformatics (ISB);

Vice Chairman and Chief of Standing Committee for the Division of Bioinformatics, Chinese Society of Interdisciplinary Sciences;

Vice Chairman, Division of the Assessment and Protection of Health &Medicine Big Data Application, Chinese Association of Health Information;

Vice Chairman and Standing Committee Member of the Division of Functional Genomics Bioinformatics and System Biology, Chinese Cell Biological Society;

Standing Committee Member of the Division of Biological Mathematics, Chinese Mathematics Society;

Executive Standing Committee Member of the Computational System Biology Division, Chinese Society of Operational Research;

Standing Committee Member of the Subdivision for Dynamic Response of Weaponry Materials, Chinese Association of Military Industries;

Ex-Member, IEEE and Engineering in Medicine and Biology Society;

Ex-Member, Biophysical Society

Ex-Member, American Chemical Society

Member, the Virtual Laboratory for Computational Chemistry of CNIC and Supercomputing Center of CNIC, Chinese Academy of Sciences

International Conferences Involved

Chaairman, AI Drug Developemt Forum, 15th "China Pharmaceutical Strategy Conference", March 18-20, 2023, Shijiazhuang, China.

Member of the Organizing Committee, "International Conference on AI and Precision Medicine Informatics & 8th National Conference on Computational Biology and Bioinformatics", May 12-15, 2023, Xuzhou, China.

Member of the Organizing Committee, " 10th National Conference on System Biology and Bioinformatics", July 22-25, 2022, Guangzhou, China.

Organizing Committee Member, "The IEEE International Conference on Bioinformatics and Biomedicine (BIBM)" , Dec. 9-12, 2021, Houston, TX, USA.

Chairman of the Organizing Committee, "International Conference on AI and Precision Medicine Informatics & 7th National Conference on Computational Biology and Bioinformatics", July 16-20, 2021, Yantai, China.

Organizing Committee Member and Session Chair, "The IEEE International Conference on Bioinformatics and Biomedicine (BIBM)", Dec. 16-20, 2020, Seoul and On-Line, Korea.

Organizing Committee Member, The 13th International Conference on Computational Systems Biology (ISB 2020), September 18-21, 2020, Haikou, China.

Member of Advisory Board, "5th Conference of Theory and Applications of Computational Chemistry (TACC2020)", September 7-12, 2020 at Hokkaido University, Sapporo, Japan.

General Chair, 16th International Symposium on Bioinformatics Research and Applications (ISBRA), December 1-4(2020), Moscow, Russia.

Organizing Committee Member, "The IEEE International Conference on Bioinformatics and Biomedicine (BIBM)", November 18-21, 2019, San Diego, CA, USA.

Organizing Committee Member,"The IEEE International Conference on Bioinformatics and Biomedicine (BIBM)", Dec 3-6, 2018, Madrid, Spain.

Member of the Program Committee, "The 13th International Conference on System Biology (ISB)", August 18-21, 2018, Guiyang, China.

Member of Organizing Committee, "17th Chinese National Conference of Interdisciplinary Sciences", Aug. 01-05, 2018, Hulunbeier, China.

Member of Organizing Committee, "10th Edition of International Conference on Structural Biology 2018", March 15-16, 2018 Barcelona, Spain.

Organizing Committee Member, "The IEEE International Conference on Bioinformatics and Biomedicine (BIBM)", November 17, 2017, Kansas City, Missouri, USA.

Organizing Committee Member, "International Conference on Proteomics (ICP-2017)", November 20-21, 2017, Rome, Italy.

Member of the Program Committee, "GIW / BIOINFO 2017 (International Joint Conference on Genome Informatics Workshop (GIW) and BIOINFO of KSBi 2017)", Oct 31-Nov 3, 2017, Seoul, South Korea.

Committee of Scientific Advisors, "The Baltic Conference Series", 08-11 October 2017, Sweden.

Chairman of Publication Committee, "Big Data Conference of Chinese Computation Federation (CCF)", October 14-16, 2017, Shenzhen, China.

Member of the Program Committee, "The 16th International Conference on Bioinformatics (InCoB 2017)", September 20-22, 2017, Shenzhen, China.

Co-Chair and Chairman of Technical Committee, "6th International Conference on Bioinformatics and Biomedical Science (ICBBS 2017)", June 22-24, 2017, Singapore.

Member of the Program Committee, "8th International Conference on Proteomics and Bioinformatics"May 22-24, 2017, Osaka, Japan.

Member of the Program Committee, "7th National Conference of Bioinformatics and System Biology", October 19-23, 2016, Chengdu, China.

Member of the Program Committee, "15th annual InCoB (International Conference on Bioinformatics)", September 21-23,2016, Singapore.

Member of the International Advisory Committee, "Theory and Applications of Computational Chemistry"-TACC 2016, Sept. 2016, Seattle, USA.

Member of Advisory Committee, "Symposium of Interdisciplinary Studies of Mathematics, Computer and Life Sciences", May 21-22, 2016, Beijing, China; Chairman, "deMon Workshop", May 4-8, Zhengzhou, China.

Chairman, "Symposium of Big Data and Precision Medicine", March 25-27, 2016, Shanghai, China.

Member of the International Advisory Committee, "International Conference on Bioinformatics and Systems Biology (BSB) ", March 4-5, Allahabad, India.

Member of the Program Committee, "The 26th annual GIW and 14th annual InCoB conference", September 9-11, 2015, Tokyo, Japan.

Member of the Program Committee, "The 9th International Conference on System Biology (ISB)", August 21-24, 2015, Luoyang, China.

Member of the Program Committee, "International Conference on Biological Engineering and Gene Technology", July 18-19, 2015, Shanghai, China.

Member of the International Advisory Board, "2nd World Congress on Biotechnology", June 2015, Hyderabad city, India.

Member of the Program Committee, The 8th International Conference on Systems Biology and the 4th Translational Bioinformatics Conference, October 25-27, 2014, Qingdao, China.

Chairman, The Oriental Forum, Sept. 28-30, 2014, Shanghai, China.

Member of Organizing Committee, The 6th National Conference of Bioinformatics and System Biology, Oct. 6-9, 2014, Nanjing, China.

Member of the Program Committee, International Conference on Bioinformatics, July 31-Aug.4, 2014, Sydney, Australia.

Member of the Program Committee, 13th International Conference on Bioinformatics of the Asia-Pacific Bioinformatics Network, July 31- Aug. 2, 2014, Sydney, Australia.

Member of the Program Committee, IEEE BIBM 2013 (The IEEE International Conference on Bioinformatics and Biomedicine), Dec. 18-21, 2013, Shanghai, China.

Chairman of the Advisory Committee, International Conference on Computational and System Biology, Nov. 14-16, 2013, Shengzhen, China, Sponsored by the International Association of Scientists in the Interdisciplinary Areas (IASIA), South University of Science and Technology of China (SUSTC) and the 2nd Hospital of Shenzhen;

Organizing Committee Member, Cell Science-2013, November 20 – 22, 2013. Baltimore, USA, organized by OMICS Publishing Group.

Member of the Program Committee, The 12th International Conference on Bioinformatics, Sept. 20-23, 2013, Taicang, Suzhou, China.

Chairman, National Symposium on Deep Carbon Circulation, July 19-24, 2013, Lushan, Jiangxi, China, Sponsored by Chinese National Geophysical Society and International Association of Scientists in the Interdisciplinary Areas (IASIA);

Member of the Program Committee, 1st International Conference on Translational Biomedical Informatics (ICTBI 2012), December 8-10, 2012, Taicang, Suzhou, China.

Chairman, International Conference on Computational and System Biology, Oct. 12-14, 2012, Shanghai, China, Sponsored by The IEEE Engineering in Medicine and Biology Society (EMBS), and International Association of Scientists in the Interdisciplinary Areas (IASIA);

Session Chair, Symposium of High-Pressure Physics, Sept. 25-27, Wuhan, China.

Vice Chairman and Session Chair, Theory and Application of Computational Chemistry, Sept. 2-7, 2012, Pavia Italy;

Session Chair, The Worldwide Chinese Computational Biology and Molecular Simulation Conference, Aug. 9-12, 2012, Dalian.

Session Chair, the 5th National Conference of Bioinformatics, Harbin, Aug. 7-10, 2012.

Chairman, 13th deMon Developer Workshop, May 11-15, 2012, Shanghai, China;

Member of Program Committee, The IEEE International Conference on Bioinformatics and Biomedicine (BIBM), Oct. 4-7, 2012, Philadelphia, USA.

Member of Program Committee, 5th National Bioinformatics Conference, Aug. 7-10, 2012, Harbin, China.

Chairman, International Conference on Computational and System Biology, Oct. 12-14, 2011, Shanghai, China, Sponsored by The IEEE Engineering in Medicine and Biology Society (EMBS), and International Association of Scientists in the Interdisciplinary Areas (IASIA);

Member of the program committee, 2011 Asian Congress of Biotechnology, May 11-15, 2011, Shanghai, China;

Chairman, International Conference on Computational and System Biology, Oct. 22-24, 2010, Hangzhou, China, Sponsored by The IEEE Engineering in Medicine and Biology Society (EMBS), and International Association of Scientists in the Interdisciplinary Areas (IASIA);

Program Chair, International Conference on Computational System Biology, Suzhou, China, Sept. 9-11, 2010, co-sponsored by National Natural Science Foundation of China (NSFC), Academy of Mathematics and Systems Sciences of CAS (AMSS), Shanghai Institutes for Biological Sciences of CAS (SIBS), Shanghai Jiao Tong University, Soochow University, Computational Systems Biology Society of ORSC, Systems Biology Technical Committee of IEEE SMC Society, and also technically sponsored by IEEE SMC Society;

Member of the program committee, The 2010 IEEE International Conference on Bioinformatics and Biomedicine, Dec. 19-22, 2010, Hong Kong;

Chairman, International Conference on Computational and System Biology, Oct. 9-11, 2009, Shanghai, China, Sponsored by The IEEE Engineering in Medicine and Biology Society (EMBS), and International Association of Scientists in the Interdisciplinary Areas (IASIA);

Member of organizing committee, The 7th International Bioinformatics Workshop, June 19th-21st, 2009, Soochow University, Suzhou, China;

Member of organizing committee, The 8th International Bioinformatics Workshop, 2010, Wuhan, China;

Chairman, Theory and Application of Computational Chemistry, Sept. 23-27, 2008, Shanghai, China, one of the largest theoretical chemistry conferences attended by 1000 scientists with 50 plenary talks;

Chairman, 2nd IEEE Conferences on Bioinformatics and Biomedical Engineering, May 16-20, 2008, Shanghai, China;

Member of the program committee, International Conference on Intelligent Data Engineering and Automated Learning (IDEAL), 2003-present

Recent Grants and Awards

1. Prediction of Drug-Target Interactions Using Graph Deep Learning and Multi-Label Learning, National Science Foundation of China, 32070662, 2021.1-2023.12, 580,000, PI.
2. Precise Clinical Positioning Decision System of Wendan Decoction, University Star Project, Shanghai Jiaotong University, The Medical-Engineering Research Funds, YG2021ZD02 2021.1-2023.12, 500,000 RMB, Co-PI.
3. Artificial Intelligence-guided Directed Evolution for Enzyme Engineering, National Science Foundation of China, 32030063, 2021.1-2024.12, 2,920,000, Co-PI.
4. Experimental Evaluation and Artificial Intelligence Design of Anti Covid-19 Drug and Vaccine, Strategic Research Funding, Guangdong Province, 2020.5-2021.12, 10 million,PI.
5. Construction of Industrial Yeast Using Artificial Intelligence Technology, Major Project, State Key Lab. Of Microbial Metabolism, Shanghai Jiaotong University, 2020.5-2022.12, 0.5 million, Co-PI.
6. Shanghai Jiaotong University(Shanghai)-Islamabad-Belgrade Antibiotics Drug Resistance Joint Creative Research Center, Science and Technology Commission of Shanghai Municipality (Grant: 19430750600), 2020.1-2023.12, 2Million, PI.
7. Fundamental Theory and Methods of High Throughput Proteomics Computation, Major Grant, National Foundation, 2.81 million, project PI, Project No: 61832019, 2019-2023.
8. The Interfacial Features and Recognition Mechanism of Protein-Protein Interactions, The Priority Area of Research, Ministry of Science and Technology, Project No.: 2016YFA0501703, 2016-2021, 4,4 million RMB, project leader.
9. Computer Aided Drug Design, First Class Course Building, Shanghai Jiaotong University, 2019.
10. Pharmacology Research and New Drug Development of Mangostin Against AD, Joint Medical-Engineering Research Funds, Shanghai Jiao Tong University, Project No. YG2017ZD14, 0.7 million, project co-leader.
11. Phase Transition of Energetic Molecular Crystals, The Challenge Research, Chinese Academy of Engineering Physics, 2016-2021, 2.8 million, project leader.
12. P450 Enzyme and Efficient Biological Synthesis of phenylpropanoic compounds, Major Project of the National Key Lab. of Microbial Metabolism, 2016-2018, 1 million, project leader.
13. The first-class awards of the national classical publication fund for <Translational Medicine Informatics>, National Funds Publication, 2016-2016, 160,000RMB, project leader.
14. The first-class international journal drives for <Interdisciplinary Sciences: Computational Life Sciences>, Shanghai High Level Journal Support Project, 2016-2016, 300,000RMB, project leader.
15. Microbial Metabolism in The Waste Treatment of Pig Farms, The National Key Technology Support Program, 2014-2016, project leader.
16. Graduate Students' Forum of Computational and System Biology, Shanghai Graduate Degree Commission, 2013-2014, project leader.
17. Software Development of Personalized Drug Design and Virtual Screening Service, National Innovation Funds, 2012-2015, project leader, project. No.238312C26213202383.
18. Fund for International Journal, Shanghai Jiao Tong University, 2013-2014, project leader.

19. Software Development For The Property Computation of Energetic Materials, Software Center, Chinese Academy of Engineering Physics, 2013-2014, project leader.
20. Joint Biophysics Lab., Shanghai Bureau of Foreign Expert, 2012-2013, project leader, project No. B2012-093.
21. Ab Initio Molecular Dynamics Simulation of Typical Explosives, National Science Foundation of China, 2012-2015, Project Leader, Project No. 11174201.
22. Multi-targets Drug Screening Technology Based on The Chinese Traditional Medicine Database, The National Research Foundation for the Doctoral Program of Higher Education of China under Grant No.20120073110057.
23. Drug Screening Technology Unifying Western and Chinese Medicine, The National High Technology Research and Development Program of China(863), 2012-2016, PI, project No.2012AA020307.
24. Fundamental and Key Problem of Synthetic Biology, The National Basic Research Program of China (973), Ministry of Science and Technology, 2012-2015, PI, project No. 2012CB721000.
25. The Major Project, Shanghai Commission of Science and Technology on The Structure of BK Channel And Molecular Mechanism Regulated by The Long Chain Fatty Acids, Prof. No: 11JC1406400,2011-2014, PI.
26. The Interdisciplinary Research Project of Shanghai Jiao Tong University on The Multi-scale Research of The Molecular Mechanism of antimicrobial peptide Mimics, 2011-2013, project leader, Project No. AE0800006.
27. Research and Development of Unified Software for SNPs of Drug-Metabolic Enzyme and Drug Response, The National High Technology Research and Development Program of China(863), 2008-2012, project leader, project No. 2007AA02Z333.
28. The National Basic Research Program of China (973) on Fundamental Durability Problems of Aerospace Devices and Equipment, Ministry of Science and Technology, 2011-2014, PI, project No. 2011CB707500.
29. The National Basic Research Program of China (973) on Fundamental and Key Problem of Artificial Vision, Ministry of Science and Technology, 2005-2014, PI, project No. 2005CB724303 and 2011CB707500.
30. Molecular Dynamics Simulation of Typical Explosives, National Key Lab. on Explosive Science and Technology, 2009-2011, Project Leader, Project No. KFJJ09-02.
31. Molecular Dynamics Simulation of Typical Explosives, National Key Lab. on Explosive Science and Technology, 2012-2014, Project Leader, Project No. KFJJ12-02.
32. Drug Discovery Technology Based on Effective Components and Multi-Targets, Ph.D. Research Funds, Ministry of Education, Project Leader, 2012-2014, project No.: 20120073110057.
33. Biophysics Joint Lab., Shanghai Bureau of Experts, 2012-2013, Project Leader.
34. Funding For International Journal of "985" Third Phase, Shanghai Jiao Tong University, 2013-2014, Project Leader.
35. Publishing Funding for "Molecular Simulation and Computer Aided Drug Design", National Publishing Funds, 2012-2013, Project Leader.
36. Major Foreign High-Level Expert Funding, National Expert Bureau, 2011-2013, Project Leader.
37. Conference Grant for the International Conference on Computational and System Biology (ICCSB, 2009), Shanghai, China, Oct. 11-13, National Science Foundation.

38. Design and Screening of Leading Compounds for Anti-Alzheimer Disease, and Relevant Theoretical Studies, National Science Foundation, 2009-2011, project leader, project No 30870476.
39. Theoretical and Computational Method and its Application of Chemical Reactions in Complex Environments, National Science Foundation, 2008-2010, project leader, project No. 20773085.
40. National Comprehensive Technology Platforms For Innovative Drug R&D, as a PI, 2009-2010, Project No. 2009ZX9301-007.
41. Conference Grant for the Theory and Application of Computational Chemistry (TACC 2008), Shanghai, China, Sept. 23-27, National Science Foundation, project leader, project No. 20810302012, 2008.
42. Conference Grant for the IEEE Bioinformatics and Biomedical Engineering, Shanghai, China, May 16-18, National Science Foundation, project leader, 2008.
43. Funding for International Journals by "985" funds from Jiao Tong University, project leader, 2008.
44. Study on the aggregation mechanism of amyloid fibrils, National Science Foundation, 2008-2011, PI, project No. 30770502.
45. Theoretical Studies of The HMX Explosives, Chinese Academy of Engineering Physics and also National Key Lab. on Explosives, 2007-2009, project leader.
46. The New Approach in Drug Design, Discoveries and Optimization of New Antibiotics Drugs, 2003-2005, Major Grant, The Tianjin Commission of Science and Technology, project leader, Project No. 033801911.
47. Discoveries and Optimization of General Anti-virus Drugs Based on Traditional Chinese Medicine Database, Major and Priority Grant from The Tianjin Commission of Science and Technology, project leader, Project No. 043185111-4, 2004-2006.
48. Design, Screening, Synthesis and Optimization of Inhibitors Against SARS, The Tianjin Commission of Education, project leader, Project No. 20030001, 2004-2006.
49. 3-D Structure Determination Using Bioinformatics, The Tianjin Commission of Science and Technology, project leader, Project No. 023618211, 2002-2005.
50. Ab Initio Molecular Dynamics Simulation of Energetic Liquids, Chinese National Science Foundation, project leader, Project No. 10376024, 2004-2006.
51. Unified Hydrophobic and Hydrophilic Potential and Its Application in The Drug Design, Chinese National Science Foundation, PI, Project No. 20373048, 2004-2006.

International Exchange Funding from Shanghai Jiao Tong University

The Grand Master Awards and Honorary Professorship on behalf of the following leading scientists:

2007,Timothy A. Springer, Harvard University, Fellow of American Academy of Sciences
Gert Lubec, Vienna Medical University, Fellow of UK Academy of Sciences

2008, Martin Karplus, Harvard University, Fellow of American Academy of Sciences
Rudolph A. Marcus, Cal. Tech, 1992 Nobel Prize in Chemistry

2010, Dennis Salahub, Univ. of Calgary, Fellow of Canadian Royal Society,
Luc Montagnier, Pasteur Institute, 2008 Nobel Prize in Medicine and Physiology

Overseas Outstanding Scholars

2010, Kuo-Chen Chou, Gordon Life Science Institute, US (ranked No. 1 in terms of hot papers) Heping Zhang, Yale University, Enrico Clemmenti, Italy.

Awards

1. The Scopus Highly Cited Scholar, 2020 and 2021.
2. The Outstanding Member Award of Shanghai Microbial Society, 2020.
3. Nomination for The First-Class Award of Natural Sciences, The Shanghai Municipal Government, 2019.
4. The Second-Class Award of the Chinese Computer Federation, 2018.
5. The Second-Class Award of Chinese Medical Society, 2017.
6. The First-Class Award of Scientific and Technological Advancement by Shanghai Municipal Government, 2017.
7. The Outstanding Ph.D. Supervisor by the Shanghai Education Commission, 2016.
8. The Science and Technology Award of Shanghai Jiao Tong University, 2013.
9. 横山亮次(Yokoyama Ryōji) Awards, 2011.
10. The Fifth MMPH Research Award, 2009
11. 2nd Prize of Scientific Advancement by CAMP, 2012 due to Screening and Drug Binding Mechanism of Anti-AIDS Drugs.
12. 2nd Prize, Excellent Undergraduate Textbook Award, Shanghai Jiao Tong University, "Molecular Simulation and Computer Aided Drug Design", 2015.
13. 2011-2012 Excellent Teacher, Shanghai Jiao Tong University
14. Nominated for the 10 Most Important Scientific Advancements 2010-2011, Ministry of Education.
15. Nominated for the Achievement in Asia Award (Robert T. Poe Prize)
16. Research Council UK for China Summer School Competition
17. Award from K.C.WONG EDUCATION FOUNDATION, Hong Kong for international conferences
18. Shanghai Mengminwei Award for 2009.
19. Shanghai Mengminwei Award for 2008.
20. 2012 "Authors Contributed the Most" to the Chinese Science Bulletin.
21. The best paper award of 2006(the first time) by <Acta Pharmaceutica Sinica> for "HIV Inhibitor Screening Based on The Traditional Chinese Medicines Database", Acta Pharmaceutica Sinica, 41(3), 241-246 (2006)(Figure was placed on the cover of the issue).
22. Shanghai Baiyulan Award for 2009.
23. Shanghai Baiyulan Award for 2006.
24. Shanghai Mengminwei Award for 2006.
25. Honorable Mention for a poster titled: "Ab Initio Molecular Dynamics Simulations of Molecular Collisions of Nitromethane", at the 12th Biennial International Conference of the APS Topical Group on Shock Compression of Condensed Matter, Atlanta, June 2001.

Major Awards received by students

26. 1. The best thesis award for undergraduate students, Beijing University to Li Lin, July 2007.
27. 2. The Morgan Stanley Award administrated by the Shanghai Jiao Tong University to Li Lin, Oct. 2007.
28. 3. The national first prize of mathematics modeling to students Liang Jianyi and Shang Yuan, Nov. 2007.
29. The National Awards For the Excellent Graduate Students awarded to Gu Ruoxiu, Dec. 2008, The DuPont Award For Graduate Students, awarded to Gu Hui, Dec. 2008.
30. The National Awards For the Excellent Graduate Students awarded to Li Li, Dec. 2010, The Jienengke 3rd Prize For Graduate Students, awarded to Chen Qi, Dec. 2009.

31. The Qiushi graduate student awards to Lian Peng, The Jienengke 2nd prize for WangYing, The Jenengke 3rd Prize for Li Li, Oct. 2011.
32. Mulan 1st Prize awarded to Gu Ruoxu, Guanghua 1st Prize to Chen Qi, Jienengke 2nd to Lian Peng, Jienengke 3rd to Li Li, Oct. 2012.
33. Shanghai Jiao Tong University-AMD High Performance Computational Awards to YukunWang. 8, 2013.
34. 9. The Outstanding Ph.D. Student to Ruoxu Gu by the Shanghai Educational Commission, 2016.
35. The Outstanding Graduate Student awarded by the Shanghai Jiaotong University, Yanjing Wang Ph.D. student, Yanjing Wang, 2018.
36. The Outstanding Graduate Student awarded by the Shanghai Jiaotong University, Yanjing Wang Ph.D. student, Chengdong Li, 2019.
37. 10.The Globalink Research Award to post-doc, Dr. Gurudeeban Selvaraj and Dr. Satyavani Kaliamurthi by the Mitacs(a national, not-for-profit organization in Canada), 2019.
38. The National Graduate Student Award to Ph.D. student, Yanyi Chu, 2020.
39. The National Graduate Student Award to Ph.D. student, Yanyi Chu, 2021.
40. The Outstanding Graduate Student awarded by the city of Shanghai to Ph.D. student, Yanyi Chu, 2022.
41. The Outstanding Undergraduate Student awarded by the city of Shanghai to Zilin Cai
42. The super postdoc awarded to Dr. Abbas Khan, 2022.
43. The city's New Researcher Award, City of Marseille and the Aix-Marseille University.

Patents

44. Dong-Qing Wei, K.C. Chou, Yiru Gan and Qishi Du, “A Polypeptide and Its Derivatives as Inhibitors Against SARS”, Patent No: CN 200410018679.3, 2005-01-05.
45. Dong-Qing Wei and Yu-Kun Ma, “Chemical synthetic methods for potential preventive and anti-Alzheimer Disease- wgx50, wgx51, wgx52, wgx180”, Patent No. ZL20111 0439656.X.
46. Dong-Qing Wei and Heng Wang, “New usage of wgx-50, an chemical extracted from Zanthoxylum Bungeanum”, 2020-06-17, Patent No. ZL202010551170.4, June 17, 2020.
47. Dong-Qing Wei and Heng Wang, “Mechanism of skin aging reversal by active ingredient WGX-50 of Zanthoxylum bungeanum Maxim”, Patent No.: 2021104838, Aug. 02, 2021.
48. Dong-Qing Wei and Heng Wang, “Extraction method of active ingredient WGX-50 from Zanthoxylum bungeanum and its application in cosmetics”, Patent No.: 2021105282, Aug. 11, 2021.
49. Dong-Qing Wei and Heng Wang, “Multi-effect Cosmetic Composition Containing Suberosin and Preparation Method thereof ”, Patent No.: 2021105695, Aug. 17, 2021.
50. Software Copy Rights
51. Molecule search software based on Maccskey V1.0, 2009SR030823, 2009.08.05
52. Database of small molecules from national products or Traditional Medicines, 2009SR042815, 2009.09.27.
53. Drug metabolism prediction software based on neural networks V1.0, 2009SR056211, 2009.12.02.
54. SNPs prediction software of CYP 450 based on SVM V1.0, 2010SR019961, 2010.05.01.
55. DNA binding sites based on protein properties, 2010R11L055771, 2010.08.09.
56. Drug metabolism prediction software based on SVM, 2010R11L055833, 2010.08.09.

57. Software obtaining the active sites of proteins, 2010R11L055755, 2010.08.09.
58. Software searching the active sites of proteins based on the Convex Hull, 2010R11L055766, 2010.08.09.
59. The database processing software to predict the SNPs based on sequences, 2010R11L055742, 2010.08.09.
60. Molecule finger-print search software based on drug molecule database, V1.0, 2010SR042160, 2010.08.18.
61. Databases of SNPs and enzymatic properties of CYP450 enzymes V1.0, 2010SR042161, 2010.08.18.
62. Database of drugs-targets and screening platform based on networks V1.0, 2010SR042163, 2010.08.18.
63. deMon Gui, V1.0, 2012SR090355.
64. Anti-cancer Vaccine Scanner (ACVA: precision based approach for cancer treatments, 2020SR0370047).
65. CytoMegaloVirus DataBase, 2020SR0249161.
66. weiBI Server, 2020SR0602725.
67. weiDOCK Server.

Highly Qualified Personal Trained

Currently supervising 6 post-doctoral fellows, 14 Ph.D. students, 9 master students; graduated 39 Ph.D. students, 61 master students, 25 post-docs. Some alumni have become quite distinguished, including Ruoxu Gu, a Tenured Associated Prof. at Shanghai Jiaotong University,Prof. Tao Zhang at Tianjin Medical University, Dr. Mingzhu Zhao and Yi Xiong at Shanghai Jiao Tong University, Peng Lian at Oakridge National Lab. Li Li at Harvard Medical School, Qi Chen at East Huadong University.

Graduate Students Supervising & Post-Doc.

Name	University	Date	Project	Status
Heqi Sun	Shanghai Jiao Tong University	2022.9	AI Drug	Ph.D. in progress
Yufang Zhang	Shanghai Jiao Tong University	2021.9	BioStat.	Ph.D. in progress
Qiankun Wang	Shanghai Jiao Tong University	2020.9	MD simulation	Ph.D. in progress
Aamir Mehmood	Shanghai Jiao Tong University	2020.9	System Biology	Ph.D. in progress
Munawar Abbas	Henan Institute of Technology	2020.9	MD simulation	Ph.D. in progress
Yitian Fang	Shagnhai Jiaotong University	2019.9	Deep learning models of diseases and biomarkers	Ph.D. in progress
Xueying Mao	Shanghai Jiao Tong University	2019.9	Deep Learning and Protein interactions	Ph.D. in progress
Arif Ali	Shanghai Jiao Tong University	2019.9	Deep Learning and Network Pharm.	Ph.D. in progress
Athar Shafiq	Shanghai Jiao Tong University	2019.9	Drug design	Ph.D. in progress

Fahad Humayun	Shanghai Jiao Tong University	2018.9	AI and Mol. Machine	Ph.D. in progress
Qiuying Dai	Shanghai Jiao Tong University	2018.9	Protein-Protein Interactions	Ph.D. in progress
Yanyi Chu	Shanghai Jiao Tong University	2017.8	Cancer Immunology	Ph.D. in progress
Ashma Sindhoo	Shanghai Jiao Tong University	2015.9	Hadoop and Network Pharmacology	Ph.D. in progress
Juan Huang	Shanghai Jiao Tong University	2015.9	Molecular Motors	Ph.D. in progress
Shenggeng Lin	Shanghai Jiao Tong University	2021.9	Deep Learning	Master in progress
Shifeng Jiang	Shanghai Jiao Tong University	2021.9	Vaccine design and AI	Master in progress
Shah Zeb Khan	Shanghai Jiao Tong University	2021.9	Vaccine design	Master in progress
Bowen Zhao	Shanghai Jiao Tong University	2020.9	Machine learning	Master in progress
Weizhi Chen	Shanghai Jiao Tong University	2020.9	MD simulation	Master in progress
Mingming Jiang	Shanghai Jiao Tong University	2020.9	Deep Learning	Master in progress
Jing Zhao	Shanghai Jiao Tong University	2020.9	Machine learning	Master in progress
Chujun Lv	Shanghai Jiao Tong University	2020.9	Machine learning	Master in progress
Zhili Zhang	Shanghai Jiao Tong University	2018.9-	Personalized Drug	Master in progress
Yatong Liu	Shanghai Jiao Tong University	2018.9	Protein Interactions	Master in progress

Students Graduated since 2005

Name	University	Date Graduated	Project	Status	Current Position
Wei Wang	Shanghai Jiao Tong University	2021.11	Research of Deep Forest Model to the Non-Coding RNA Omics Data	Ph.D.	Takeda Pharma.
Abbas Khan	Shanghai Jiao Tong University	2021.11	Structure-based approaches to understand the molecular mechanism	Ph.D.	Shenzhen institute of Advance Technology,

			of pathogenesis and development of therapeutics database for human respiratory viruses		Chinese Academy of Sciences
Taimoor Khan	Shanghai Jiao Tong University	2021.11	Development of biological databases and its application in designing therapeutics against human pathogenic viruses	Ph.D. in progress	Shenzhen institute of Advance Technology, Chinese Academy of Sciences
Yanjing Wang	Shanghai Jiao Tong University	2019.9-	Molecular Simulation, Drug Design, Molecular Docking	PhD	Post-doc at Shanghai Jiao Tong University
Mahamma d Junaid	Shanghai Jiao Tong University	2020.3	Deep Learning an Cancer Immunity	PhD	Shenzhen institute of advance technology
Chengdong Li	Shanghai Jiao Tong University	2020.3	MD Simulations of Membrane Proteins	Ph.D.	Fujian medical University
Fang Li	Shanghai Jiao Tong University	2019.12-	MD Simulations of Protein Clusters	Ph.D.	Shanghai Jiao Tong University
Yuxin Du	Shanghai Jiao Tong University	2019.9-	Acute Myeloid Leukemia	Ph.D.	Najing Hospital
Kening Li	Shanghai Jiao Tong University	2019.9-	Acute Myeloid Leukemia	Ph.D.	Nanjing medical University
Xiaoqing Guan	Shanghai Jiao Tong University	2019.6	Membrane Permeation	Ph.D.	Shanghai University of Chinese Traditional Medicine
Chunwei Leng	Wuhan Institute of Tech.	2019.7	Energetic Materials	Ph.D.	Henan Institute of Technology
Xiuqing Zhang	Sichuan University	2018.7	High-energetic co-crystal explosive CL-20/TNT	Ph.D.	Zhongbei University

Huiyuan Zhang	Shanghai Jiao Tong University	2018.7	Simulation of Membrane and Protein	Ph.D.	Hebei University of Railways
Yanzhi Bai	Shanghai Jiao Tong University	2018.7	High-pressure Solid CO2 Single-crystal Diffraction and Theoretical Studies	Ph.D.	Post. doc Shanghai Jiao Tong University
Huaimeng Fan	Shanghai Jiao Tong University	2017.7	AD and Wgx-50	Ph.D.	Suzhou Investment Co.
Hao Dai	Shanghai Jiao Tong University	2017.6	Statistical Modeling of CYP 450 Metabolism	Ph.D.	Shanghai Academy of Biological Sciences
Yuanyuan Qi	Sichuan University	2016.7	Condensed Matter Physics	Ph.D.	Henan University of Technology
Yukun Wang	Shanghai Jiao Tong University	2015.7-	New Algorithm of Free Energy Calculation Membrane Permeation Mechanism of Antimicrobial Peptides	Ph.D.	Post.doc at Yale University John Hopkins University
Li Zhang	Beijing Institute of Technology	2015.7	Applied Physics	Ph.D.	Post-doc at Beijing Institute of Technology
Shouxin Cui	Shanghai Jiao Tong University	2015.5-	Theoretical Study of TiZr Alloys	Ph.D.	Liaocheng University
Nina Ge	Sichuan University	2011.7-	Energetic Materials	Ph.D	Xinan University of Science and Technology
Kai Xu	Sichuan University	2010.7-	Energetic Materials	Ph.D.	Henan University Hydro-Power
Peng Lian	Shanghai Jiao Tong University	2013.11	Hybrid Quantum Mechanics and Molecular Mechanics; Drug Metabolism and Cytochrome P450 enzymes; The Catalytic Mechanism of Cellulase	Ph.D.	Fudan University
Ruoxu Gu	Shanghai Jiao Tong University	2013.11	Molecular Dynamics Simulation of M2 Channel	Ph.D.	Post Doc. Oakridge National Lab. USA

Chen Qi	Shanghai Jiao Tong University	2013.11	Impact of resistance mutations on inhibitor binding to HIV-1 integrase	Ph.D.	East China University of Science and Technology
Li Li	Shanghai Jiao Tong University	2013.6	Study of SNPS in Human Cytochrome P450 and Protein-Chemical Interactions	Ph.D.	Post-doc in Harvard Medical School
Mingzhu Zhao	Shanghai Jiao Tong University	2013.6	Study on Predictions of Drug-Target Interactions And Drug Combinations	Ph.D.	Shanghai Jiao Tong University
Ying Wang	Shanghai Jiao Tong University	2012.6	Study on Structure and Function of Two Kinds of Important Proteins Based on MD Simulation	Ph.D.	Shanghai Academy of Agricultural Sciences
Xiaoli Yuan	Sichuan University	2012.5	Theoretical Study on Elastic, Electronic Structure and Thermodynamic Properties of Zr Alloy	Ph.D.	Hehai University
Hongling Cui	Sichuan University	2011.7	Ab Initio Studies of HMX	Ph.D.	Henan Industrial University
Tao Zhang	Shanghai Jiao Tong University	2011.7	CYP-nsSNP Database and Theoretical Study of Cyp-mediated Drug Metabolism	Ph.D.	Tianjin Medical University
Yi Xiong	Wuhan University	2011.5	The Study of Characterization and Prediction of Binding Sites on Proteins Based on Machine Learning Methods	Ph.D.	Assistant Professor at Shanghai Jiao Tong University, China
Jing Chang	Sichuan University	2010.10	First-principles MD Simulations of Solid NM and β-HMX	Ph.D.	Sichuan Normal University
Yanli Zhang	Southwest Jiao Tong University	2010.7	Mesoscopic Simulation of Aggregate Behavior of Fluoropolymers in the TATB-Based PBX	Ph.D.	Leshan College
Hong Liu	Southwest Jiao Tong University	2009.7	Ab Initio MD Simulations of Nitromethane Liquids	Ph.D.	China Earthquake Research Institute

Laiyu Lu	Sichuan University	2009.7	Ab Initio Studies of HMX	Ph.D.	Sichuan Normal University
Jingfang Wang	Shanghai Institutes for Biological Sciences	2009.7	Molecular Dynamics Simulations of CYP450 SNPs	Ph.D.	Shanghai Jiao Tong University
Xiaoli Guo	Shanghai Jiao Tong University	2008.7	Cleavage Mechanism of the H5N1 Hemagglutinin by Trypsin and Furin	Ph.D.	Shanghai Jiao Tong University
Zhiwen Shi	Shanghai Jiao Tong University	2021.7-	Protein Machine	M.Ms.	A company in Chengdu
Bin Han	Guangzhou University of Chinese Medicine	2020.7	Gene Expression	M.Sc.	A Guangzhou company
Yufang Zhang	Shanghai Jiao Tong University	2019.7	Deep learning	M.Sc.	Shanghai Investment company
Xiangen Wang	Shanghai Jiao Tong University	2019.7	Muti-label	M.Sc.	PhD at City university of Hongkong
Xiaoqi Shan	Shanghai Jiao Tong University	2019.7	Drug Combination	M.Sc.	Qunar.com
Ali Arif	Shanghai Jiao Tong University	2019.7	Design of validated vaccines against Epstein-Barr virus (EBV)	M.Sc.	Shanghai Jiao Tong University
Qiankun Wang	Shanghai Jiao Tong University	2019.7	MD Simulations of Proteins	M. Sc.	Shanghai Jiao Tong University
Siying Qu	Shanghai Jiao Tong University	2019.7	Drug Design	M.Sc.	Huawei
Abbas Khan	Shanghai Jiao Tong University	2018.9	Identification of novel drug targets against Diamond-Blackfan anemia	M.Sc.	Shanghai Jiao Tong University
Shuang Hou	Shanghai Jiao Tong University	2015.7-	Inhibition of β-amyloid Channels	M.Sc.	PhD in Tongji university

Zhenhua Li	Shanghai Jiao Tong University	2016.9	MD Simulations of Membrane Proteins	M.Sc.	An accounting firm
Liyue Bai	Shanghai Jiao Tong University	2015.7-	Drug Combinations by an Improved Naïve Bayesian Algorithm	M.Sc	An investment Company
Qian Xu	Shanghai Jiao Tong University	2018.9-	Drug Combination	M.Sc.	Lily Shanghai
Haifeng Yang	Shanghai Jiao Tong University	2018.7	Drug Combinations	M.Sc.	Huawei, Hangzhou
Pan Tan	Shanghai Jiao Tong University	2018.7	MD Simulations	M.Sc.	Shanghai Jiao Tong University
Yuxi Zheng	Shanghai Jiao Tong University	2016.9-	Personal Drug	M.Sc.	Self-employed
Yiqing Wei	Shanghai Jiao Tong University	2015.7-	Genetic Islands	M.Sc.	Sina.com
Tangzhen Zhao	Shanghai Jiao Tong University	2014.7-	MD Simulation of Membrane Proteins	M.Sc.	Ph.D. Studies at Shanghai Jiao Tong Univ.
Yifan Sun	Shanghai Jiao Tong University	2014.7	Drug Combination Prediction	M.Sc.	Novartis
Jianping Lv	Shanghai Jiao Tong University	2014.7	Molecular Dynamics Simulation on Proteins	M.Sc.	GM Shanghai
Lin Huang	Shanghai Jiao Tong University	2013.7	Molecular Dynamics Simulation of M2 from Influenza A Virus	M.Sc.	Royal Institute of Technology Roslagstullsbacken 15 SE-10691 Stockholm, Sweden
Chaohui Jin	Shanghai Jiao Tong University	2013.4	Integration of Cyp450 Metabolism Database and Online Prediction of Compound Adme	M.Sc.	Self-employed
Shigao Chen	Shanghai Jiao Tong University	2012.7	Virtual Screening for New Drug Candidates Against Alzheimer's Disease Based on Stitch Database	M.Sc.	Patent Bureau Suzhou

Peisi He	Shanghai Jiao Tong University	2012.7	The Molecular Dynamics Simulation Study of Influenza Virus B Proton Channel	M.Sc.	Siemens Power
Quanyi Li	Shanghai Jiao Tong University	2012.7	High-pressure Solid CO2 Single-crystal Diffraction and Theoretical Studies	M. Sc.	
Juan Liang	Shanghai Jiao Tong University	2012.7	MD Simulations	M.Sc.	Novartis Shanghai
Yanyan Qin	Shanghai Jiao Tong University	2012.7	Quantum Studies of Nitromethane	M.Sc.	
Yufang Wang	Shanghai Jiao Tong University	2012.7	Study of the Functional Consequences of Single Amino-acid Substitution in Human Cytochrome p450	M.Sc.	Stockholm University
Qiang Zhou	Shanghai Jiao Tong University	2012.7	Prediction of Protein-ligand Interaction Based on Chemical Preference & Construction of Human Cytochrome P450 Substrate Database (CYP-Meta)	M.Sc.	Sina, Beijing
Xiaobing Li	Wuhan University	2012.5	MD Simulations	M.Sc.	
Yilei Wen	Institute of Animal Science, Academia Sinica	2012.5	Statistical Modeling	M.Sc.	
Chaoqun Xu	Liaoning University	2012.4	Hypervelocity Impact Simulation of TC4 Alloy Based on Material Point Method	M.Sc.	Dongling Vibration Test Instrument Co., Ltd
Jian Yang	Liaoning University	2012.4	Energetic Materials	M.Sc.	
Jiao Zhang	Liaoning University	2012.4	Ferroelectric Liquid Crystals	M.Sc.	
Xiaolei Cui	Liaoning University	2011.12	Energy Materials	M.Sc.	

Jing He	Shanghai Jiao Tong University	2011.7	Prediction of the Protein-Ligand Binding Sites Based on Geometric Algorithm and Evolutionary Sequence Conservation	M.Sc.	Shanghai Data
Jue Li	Shanghai Jiao Tong University	2011.7	Investigations of Drug-metabolized Enzyme Cytochrome p450 and their Implications for Personalized Drug—Drug-Metabolized Mechanism of CYP2E1	M.Sc.	Shanghai Auto Desk
Huimin Lv	Shanghai Jiao Tong University	2011.7	Free Energy Calculations and Binding Analysis of Two Potential Anti-Influenza Drugs with Polymerase Basic Protein-2 (pb2)	M.Sc.	Pfizer Shanghai
Zhaobin Xu	Shandong University	2011.7	Zinc Finger Stimulation and Optimization	M.Sc.	Villanova University
Liwei Yan	Liaoning University	2011.7	Ferroelectric Liquids	M.Sc.	
Yu Yao	Shanghai Jiao Tong University	2011.7	Mutation Probability of Cytochrome p450 Based on Ga-svm	M.Sc.	Pfizer Shanghai
Lin Gao	Liaoning University	2010.7	Ferroelectric Liquids	M.Sc.	
Shuo Liu	Liaoning University	2010.7	Studies of HMX Using Different Force Fields	M.Sc.	
Zhiyuan Xie	Shanghai Jiao Tong University	2010.7	The Computational Model to Predict Accurately Inhibitory Activity for Inhibitors towards CYP3A4.	M.Sc.	BIG
Congying Dai	Henan Normal University	2010.6	Theoretical Studies of the Rate of Excited State Proton Transfer	M.Sc.	Nantong Cambridge International Exam Center
Hui Gu	Shanghai Jiao Tong	2009.7	Research on HIV-1 Protease Drug	M.Sc.	Ph.D in Rutgers University, USA

	University		Resistance and Virtual screening for Possible Drug Candidates for Alzheimer's Disease.		
Xinchi Hou	Liaoning University	2009.7	CYP 450 Database	M.Sc.	University of British Columbia
Jihe Hu	Liaoning University	2009.7	Ferroelectric Liquids	M.Sc.	Philips
Dan Lian	Liaoning University	2009.7	LDA Studies of HMX	M.Sc.	
Xijun Wang	Shanghai Jiao Tong University	2009.7	Detonation Mechanism of Energetic Materials Using First Principle Modeling	Researcher/M.Sc.	Concordia University, Canada
Bei Tang	Shanghai Jiao Tong University	2008.7	MD Simulations	M.Sc.	Siemens Hong Zhou
Lu Wang	Liaoning university	2007.8	Ab Initio Studies of Al Clusters	M.Sc.	Hong Poly-tech University
Yingjie Wang	Liaoning university	2007.8	Effect of Dipole Elongation on the Ferroelectric Phases of Polar Liquids	M.Sc.	
Yun Li	Tianjin Normal University	2007.7	3-D QSAR of Anti-Bacterial Molecules	M.Sc.	Tianjin Police School
Huachun Wei	Tianjin Normal University	2007.7	Molecular Insights of SAH Enzyme Catalysis and Implication for Inhibitor Design	M.Sc.	Tianjin Industrial University
Rui Zhang	Tianjin Normal University	2007.7	Drug Design against SARS	M.Sc.	University of Calgary
Huiqin Zheng	Tianjin Normal University	2007.7	Screening for New Agonists against Alzheimer’s Disease	M.Sc.	Henan Educational College
Chunfang Wang	Tianjin Normal University	2007.7	Structure and Vibrational Frequencies of Ph3PCl2 With Discrete Solvent Molecules and in Gas Phase	M.Sc.	Tianjin High School

Hui Gao	Tianjin Normal University	2006.7	QSAR of HIV Drug Candidates from the Traditional Medicine	M.Sc.	Zhejiang University
Weina Gao	Tianjin Normal University	2006.7	Agaritine and Its Derivatives Are Potential Inhibitors against HIV Proteases	M.Sc.	
Shuqing Wang	Tianjin Normal University	2006.7	Cleavable Peptides of SARSCoV Mpro and Chemical Modification of Octapeptides	M.Sc.	Tianjin Medical University
Wenkang Di	Shanghai Jiao Tong University	2021.7	Deep learning and microbiology	B.S.	Shanghai Jiao Tong University
Tianhang Chen	Shanghai Jiao Tong University	2021.7	Type IV secreted effectors	B.S.	Shanghai Jiaotong University
Lifeng Zhang	Ottawa University	2020.8	Summer Student	B.S.	Oaatwa Univ.
Tongwei Dai	Shanghai Jiaotong University	2020.7	HLA epitope	B.S.	Shanghai Jiaotong University
Yi Fang	Shanghai Jiaotong University	2020.7	Antimicrobial peptides	B.S.	Shanghai Jiaotong University
Kejia Liu	University of California, Santa Barbara	2020.8	Stat. and diseases	Summer students	University of California, Santa Barbara
Mengyang Li	Shanghai Jiaotong Univ.	2020.8	Deep Learning	B.S.	Shanghai Jiaotong Univ.
Yi Lai	Chinese Univ. of Agriculture	2019.8	Stat. Models	Summer student	University of Wisconsin
Zhennan Peng	Lanzhou University	2019.8	Deep Learning	Summer student	Zhongshan University
Vicent Clark	Ottawa University	2018.9	MD simulations of antimicrobiald peptides	Summer students	Ottawa Univ.
Wenhan Chang	Shanghai Jiao Tong University	2014.7-	MD Simulations	Undergraduate	Ph.D. in US
Zhuofei Meng	Shanghai Jiao Tong University	2014.7-	MD Simulations	Undergraduate	Ph.D. in US

Junqiang Jiang	Zhengzhou Information Engineering University	2012.9	DeMon GUI	B.Sc.	A company in Wuhan
Songyao Ma	Shanghai Jiao Tong University	2013.7	Construction and Analysis of Extremophile Gene Database	B.Sc.	Graduate Studies in US
Xiaolin Hu	Shanghai Jiao Tong University	2013.7	The mechanism of Pyrococcus furiosus RecJ interac with ssDNA/ssRNA	B.Sc.	Shanghai Jiao Tong University
Yiwei Zhou	Shanghai Jiao Tong University	2013.7	Virtual Screening of New Drug Target on G-Protein Coupled Receptor Based on Statistical Models	B.Sc.	Academia Sinica
Huiying Yan	Shanghai Jiao Tong University	2013.7	MD Simulation Study of the M2 Proton Channel of Influenza Virus B	B.Sc.	Shanghai Jiao Tong University
Qian Cheng	Shanghai Jiao Tong University	2012.7	Metabolic Database of CYP450	B.Sc.	University of Michigan
Hao Zhang	Shanghai Jiao Tong University	2012.7	MD simulation of Amyloids	B.Sc.	Duke University
Qing Zhao	Shanghai Jiao Tong University	2011.7	Bioinformatics Studies of CYP 450	B.Sc.	Yale University
Detian Deng	Shanghai Jiao Tong University	2011.7	The Application of Bayesian Classification Method to Clinical Diagnosis and Prognosis	B.Sc.	Johns Hopkins University
Jiaqi Wu	Shanghai Jiao Tong University	2011.7	Active ingredients based on traditional Chinese medicine and multi-target drug molecule screening	B.Sc.	Taiwan
Leyan Chu	Shanghai Jiao Tong University	2010.10	Multi-Scale Modeling of Mucosal Cancer and Photodynamic Therapy	B.Sc.	MF in progress

Ge Gong	Shanghai Jiao Tong University	2010.7	MD simulations of FXA	B.Sc.	University of Southern California
Pengfei Liu	Wuhan University of Technology	2010.3	Modulation of the Spontaneous Curvature and Bending Rigidity of Lipid Membranes by Interfacially Adsorbed Amphipathic Peptides	B.Sc.	Suzhou Feng hua Environmental Engineering Co.,Ltd.
Roujie Chen	Shanghai Jiao Tong University	2009.7	CYP450 and Absorption, Distribution, Metabolism and Excretion (ADME) of drug molecules	B.Sc.	Columbia University
Yuan Shang	Shanghai Jiao Tong University	2009.7	Research of Substrate Selectivity A Mutant of Candida Antarctica Lipase B	B.Sc.	Hong Kong University of Science and Technology
Jianyi Liang	Shanghai Jiao Tong University	2009.7	Chinese Traditional Medicine Database	B.Sc.	Shanghai Jiao Tong University
Runfa Wu	Shanghai Jiao Tong University	2009.7	DNA-S Modification	B.Sc.	Graduate Studies in US
Yao Zhou	Shanghai Jiao Tong University	2009.7	Theoretical Studies of CYP450 Enzyme	B.Sc.	Shanghai Jiao Tong University
Binglin Yue	Shanghai Jiao Tong University	2009.7	MD Studies of Anti-Bacteria Peptides	B.Sc.	Graduate Studies in US
Jingyi Yan	Shanghai Jiao Tong University	2009.7	MD Simulation of CYP1E2	B.Sc.	University of British Columbia
Chengchen g Zhang	Shanghai Jiao Tong University	2009.7	MD Simulation of CYP1D6	B.Sc.	University of British Columbia
Yuqing Zhong	Zhengzhou University	2009.7	Biomedical Engineering, Electro-Neurophysiology	B.Sc.	University of North Texas
Mengchen Pu	Shanghai Jiao Tong University	2008.7	SNP Prediction of CYP450	B.Sc.	Graduate studies in Europe

Jisi Tang	Shanghai Jiao Tong University	2008.7	MD Simulation of CYP3A4	B.Sc.	Boston University
Shuhao Yu	Shanghai Jiao Tong University	2008.7	Neural Network Modeling and QSAR	B.Sc.	Institute of Biological Sciences, Academia Sinica
Yuanli Zhang	Northwest University	2008.7	QM/MM Studies of Enzyme Catalysis	B.Sc.	University of Oklahoma
He Zhang	Shanghai Jiao Tong University	2007.7	MD Simulations of Water Channels	B.Sc.	University of Wisconsin
Tianhang Chen	Shanghai Jiao Tong University	2021.9	Machine learning		undergraduate student

Visiting Scholars/Post-Doc.

Name	Institutions	Duration	Field of Studies	Degree	Professional Title
Xuan Xiao	Jingdezhen College	2007-2008	Bioinformatics	Ph.D.	Professor
Aixiu Li	Chinese Air Force Medical University	2007-2008	Computer Aided Drug Design	Ph.D.	Professor
Yongxiang Shi	Shandong University	2009-2010	MD Simulation of Protein-DNA Interactions	Ph.D.	Associate Professor
Wencheng Li	South China Institute of Technology	2007-2008	Bioinformatics	Ph.D.	Post-doc Fellow
Bin Wang	Anhui Medical University	2012-2013	Biostatistics	Ph.D.	Associate Professor
Guangfu Ji	Chinese Academy of Engineering Physics	2012-2013	Condensed Matter Physics	Ph.D.	Professor
Fenglei Yang	Shanghai University	2012-2013	Bioinformatics	Ph.D.	Lecturer
Linjing Zhao	Shanghai Technical University	2012-2013	Bioinformatics	M.Sc.	Lecturer
Tiantian Li	Guizhou College of Chinese Medicine	2012-2013	Computer Aided Drug Design	M. Sc.	Lecturer
Yonghong Zhang	Chongqing Medical College	2014-2015	Computer Aided Drug Design	Ph.D.	Lecturer

Bo Zhou	Guizhou Medical College	2014-2015	Computer Aided Drug Design	Ph.D.	Associated Professor
Diaxi Li	Shanghai University of Science and Technology	2015-2016	MD Simulation of Thermo-stability of Protein	Ph.D.	Associated Professor
Meena Kumari	Shanghai Jiao Tong University	2015-2017	Drug Combination	Ph.D.	Post-Doc
Faez Iqbal Khan	Henan Institute of Technology	2015-2017	MD Simulation of Protein Catalysis	Ph.D.	Post-Doc
Yongkai Wei	Henan Institute of Technology	2015-	Ab initio MD of Energetic Materials	Ph.D.	Research Assistant Professor
Yuanyuan Qi	Henan Institute of Technology	2016-	Thermal Transportation	Ph.D.	Research Assistant Professor
Kotb Attia	Shanghai Jiao Tong University	2015-2016	Personalized Drug Design	Ph.D.	Post-Doc
Ran Huang	The University of Akron	2015-2020	Polymer Modeling	Ph.D.	Post-Doc
Gurudeeban Selvaraj	Henan Institute of Technology	2017-	Cancer Immunology	Ph.D.	Post-Doc
SatyavaniKaliamurthi	Henan Institute of Technology	2017-	Cancer Immunology	Ph.D.	Post-Doc
Aman Chandra Kaushik	Shanghai Jiao Tong University	2017-2021	Protein-Protein Interaction	Ph.D.	Post-Doc.
Muhammad Tahir Khan	Shanghai Jiao Tong University	2018-2020	Microbiology and Tuberculosis	Ph.D.	Post-Doc.
Heng Wang	Shanghai Jiao Tong University	2018-2021	Synthetic Biology	Ph.D.	Post-Doc
Sathishkumar Chinnasamy	Shanghai Jiao Tong University	2018-2021	CADD	Ph.D.	Post-Doc
Yanjing Wang	Shanghai Jiao Tong University	2019-2021	CADD	Ph.D.	Post-Doc
Xue Jiang	Shanghai Jiaotong University	2020-	Single cell biology	Ph.D.	Post-Doc
Abbas Khan	Institute of AdvancedStudies, Chinese Academy of Sciences	2021-	AI drugs	PhD	Post-doc
Taimoor Khan	Institute of AdvancedStudies, Chinese Academy of Sciences	2021-	AI cancer	Ph.D.	Post-doc

Muhammad Suleman	Shanghai Jiaotong University	2019-2022	Covid-19	Ph.D.	Post-doc