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.
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Scientific Publications

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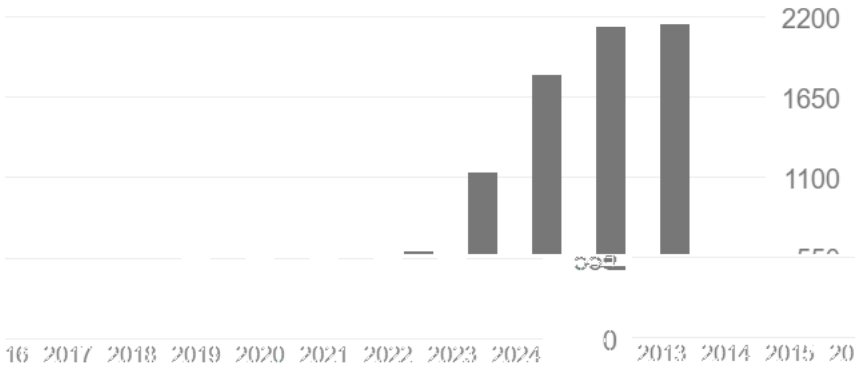

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5. Dong-Qing Wei, Intelligence Supercomputing Precision Drug Discovery: Anti-Aging and COVID- High-Performance Computing and Artificial Intelligence Technology Symposium, June 17, 2021, A nationwide conference organized by ACM SIGHPC CHINA, School of Information Science and Engineering, Hunan University, National Supercomputing Changsha Center at Changsha, Hunan.

6. Dong-Qing Wei, and drug candidates by super- "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, and drug candidates by super- The 16th International Congress of Genomics, October 25-31, 2021, A global conference organized by BGI, The China National GeneBank (CNGB), GigaScience at Qingdao.
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18. Dong-Qing Wei, 18th nationwide Yangtze River Delta Science and Technology 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, nationwide China Biomedical Technology Innovation and Development Summit Forum and the Second Xiangjiang Academician Forum 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, nationwide 2021 High-Performance Computing and Artificial Intelligence Technology 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, nationwide 8th "From Atoms to Earth" Symposium on High-Pressure Science and Earth 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, nationwide invited Symposium on Protein Structure Prediction Based on Next-Generation Supercomputing 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, bilateral Biorefining and Synthetic Biology" China-Thailand Cooperation and Exchange 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, nationwide Medical Mathematics Satellite Academic participation organized by the Medical Mathematics Committee of the Chinese Mathematical Society on October 24th, 2021 at Kunming, Yunnan.
25. Dong-Qing Wei, nationwide 10th National Conference on Bioinformatics and Systems Invited breakout sessions organized by the Chinese Society of Bioinformatics from October 25-28, 2021 at Chengdu.
26. Dong-Qing Wei, 14th nationwide Annual Conference of the Chinese Society of Biological 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, nationwide 2021 3rd China Active Health organized by China Active Health Innovation Alliance, Beijing Precision Medicine Society from October 22-24, 2021 at Shanghai.

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31. Dong-Qing Wei, fourth nationwide conference on Computational and Mathematical Bioinformatics and B organized by TSIMF from December 13-17, 2021 at Sanya, Hainan.
32. Dong-Qing Wei, 11th nationwide Jiangsu Provincial Conference on organized by Bioinformatics Professional Committee of Jiangsu Biomedical Engineering Society from December 04-05, 2021 at Nanking.
33. Dong-Qing Wei, nationwide Wu Wenjun Artificial Intelligence Science and Technology Award 10th Anniversary Award Ceremony and 2020 Chinese Intelligent Industry Annual attended invited breakout sessions organized by the Chinese Society of Intelligent Engineering from April 10-12th 2021 at Suzhou.
34. Dong-Qing Wei, Intelligence Supercomputing and Accurate Drug 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, Intelligence Supercomputing and Accurate Drug Supercomputing and AI-assisted COVID-19 Prevention and Cure, Aug. 28, 2020, Online Conference, invited talk.
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69. Dong-Qing Wei, Event Dynamics of Ion Permeation Across Membranes and Theory and Application of Computational Chemistry, Seattle, USA, August 13-September 5, 2016.
70. Dong-Qing Wei, Improved Feature-Based Approach to Predict Effective Drug Invited Talk at the 10th International Conference on Systems Biology, Weihai, China, August 19-22, 2016.
71. Dong-Qing Wei, Medicine Plenary Talk at the 16th National Conference of Interdisciplinary Sciences, Dandong, China, August 5-8, 2016.

72. Dong-Qing Wei, of CYP450 and Molec
National Conference of Microbial Genetics, Hob
73. Dong-Qing Wei, of CYP450and Molec
the6th Agricultural Microbiology, 15th Insect
Shanghai, China, July 17-19, 2016.
74. Dong-Qing Wei, Energy Calcula
Shanghai Workshop on Frontiers in Mole
75. Dong-Qing, Wei, Studies
International Workshop on Quantum
XXI) Vancouver, Canada, July 2-9, 2
76. Dong-Qing Wei, of CYP45
the 2016 Cross-Strait Predictive
Taichung, Taiwan, May 5-7, 201
77. Dong-Qing Wei, Initio M
the International Workshop M
78. Dong-Qing Wei,
Conference of Big Data an
79. Dong-Qing Wei,
Performance Computin
80. Dong-Qing Wei,
in The Geophysical
Pressure Geophysic
81. Dong-Qing Wei,
[redacted]
Plenary Talk
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82. Yukun War
Systems a
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87. Dong-Qing Wei, and Chemistry of Deep Carbon Plenary Talk at the 3rd National Conferences on Geo-biochemistry, Wuhan, China, March 17-18, 2015.
88. Dong-Qing Wei, Drug Candidate from Traditional Chinese Medicine and Its Potential Role Against AD And in Anti- 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, Event Dynamics: Ion Transportation Through Protein channels and Across Membranes and 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, Energy Calculation For Membrane Systems and 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, Studies of Carbon Circulation- Chemical Reactions of Systems Consists of C, H, N, O in The High-Pressure Regime, And Solid Phases of Carbon Plenary talk at The Oriental Forum, Shanghai, China, Sept. 28-30, 2014.
92. Yukun Wang, Ruoxu Gu and Dong-Qing Wei, Event Dynamics: Ion Transportation Through Protein channels and Across Membranes and Plenary Talk at 14thNational Conference of Interdisciplinary Sciences, Zhengzhou, China, Sept. Aug. 7-

0.000008871 0 595.32 841.92 reW* nBT/F2 11.04 Tf1 0 0 1 488.26 553.21 Tm0 0 GT(1)

100. Li Li, Hai Dai and Dong-Qing Wei, Studies of CYP450 SNPs and Personalized Drug 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, to deMon-GUI and QM/MM Studies of Enzyme Catalytic Re Plenary Talk at deMon workshop, Toulouse, France, June 20-24, 2013.
102. Dong-Qing Wei, Kai Xu, Yanzhi Bai, Shouxin Cui and Guangfu Ji, Studies of Carbon Circulation- Chemical Reactions of Systems Consists ofC, H, N, O in The High Pressure Regime, And Solid Phases of Carbon 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, Event Dynamics and Its Applications on the Free Energy Calculations for Membrane Protein Invited talk at the Theory and Application of Computational Chemistry (TACC 2012), Pavia, Italy, Sept. 1-8, 2012.
104. Dong-Qing Wei,

114. Dong-Qing Wei, Mechanism of Solid Plenary talk at The National Conference on Dynamics Response, Tianyuan, China, July 2011.
115. Dong-Qing Wei, Bioinformatics, Traditional Chinese Medicine Database (TCMD) and Personalised Drug Asian Biotechnology Congress, May 11-15, Shanghai, China, Invited talk.
116. Dong-QingWei, Chemistry for Some Real Chemical and Biological Plenary talk at deMon Workshop, Bremen, Germany, June 2011.
117. Dong-Qing Wei, Chemistry For Some Real Chem/Bio Problems: Reaction Mechanism of Explosives, Personalized Drug Design, Membrane Proteins and Protein-DNA Indian Theoretical Chemistry Symposium, Dec. 8-12, Kanpur, India, plenary talk.
118. Dong-Qing Wei, Bioinformatics For Real Biological Problems: Personalized Drug Design, Membrane Proteins And The Protein-DNA 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, Bioinformatics, Traditional Chinese Medicine Database (TCMD) and Personalized Drug 2008 Analysis of Effective Components of Chinese Traditional Medicines, Haikou, Nov. 11-13, 2009, plenary talk.
120. Dong-Qing Wei, Bioinformatics, Traditional Chinese Medicine Database (TCMD) and Personalized Drug 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, Bioinformatics, Traditional Chinese Medicine Database (TCMD) and Personalized Drug Recand Progress in Computer Simulations in Molecular Progress Sciences, Seoul, Korea, June 14-16, 2009, plenary talk.
122. Dong-Qing Wei, Bioinformatics, Traditional Chinese Medicine Database (TCMD) and Personalized Drug Westlake International Conference on Personalized Medicine, [redacted]
123. Dong-Qing Wei, Bioinformatics, Traditional Chinese Medicine Database (TCMD) and Personalized Drug 2008 World Congress on Personalized Medicine, Fushan, Oct. 5-7 2008, invited talk.
124. Dong-Qing Wei, Bioinformatics, Traditional Chinese Medicine Database (TCMD) and Personalized Drug 2008 Effective Components of Chinese Traditional Medicines, Shenzhen, Oct.

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128. Lin Li and Dong-Qing Wei, of Drugs Using Computer Aided Drug Design 10th International Congress on Amino Acids and Proteins, Chalkidiki, Greece, August 2007 (invited talk).
129. Jing-fang Wang and Dong-Qing Wei, Modeling of CYP450 and Personalized Drug 9th Computational Conference of Chinese Chemical Society, Chengdu, Aug. 2007.
130. Dong-Qing Wei, Aided Drug Design Against HIV Based on Traditional Chinese Medicine World AIDS Day, Tianjin, Nov. 2006 (invited talk).
131.
132. Dong-Qing Wei, Design Against International Symposium for Chinese Medicinal Chemists, ISCMC, Nanjing, October 2006(invited talk).
133. Dong-Qing Wei, and Inhibitor Design Against 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, and Its Application on Inhibitor Design Against 3rd International Symposium Computational Methods in Toxicology and Pharmacology Integrating Internet Resources (CMTPI-2005), Shanghai, Oct. 2005.
136. Dong-Qing Wei and Qishi Du, Combined Study of Ab Initio Quantum Mechanics and Integral Equation Theory in Three- 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 of the SARS drug and other research, Chinese Chemical Societies, Changsha, P.R. China, April 2004 (invited talk).
138. Dong-Qing Wei, invited talk, And Its Application to Drug Design Against International Conference on Theory and Application of Computational Chemistry (TACC), Geonjiu, Korea, Feb. 2004(invited talk).
139. Dong-Qing Wei, plenary talk, initio Molecular Dynamics Simulations of Molecular 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, Initio Studies of Organic Molecular 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 Progress in Metallic Hydrogen Xiamen, P.R. China, Nov. 2004.
142. Rui Zhang, Yu Ji, Aixiu Li, Xin Zhang, Qishi Du, Kuo-Chen Chou, and Dong-Qing Wei, and Docking Studies of the SARS-CoV Mpro binding with a few 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, QM/MM and Ab Initio Molecular Dynamics of Nitromethane at High in International Detonation San Diego, 2002.

144. Dong-Qing Wei, F. Zhang and T. K. Woo, -Principle Simulations of Energetic Molecular in Wave 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", Problems of Solvation and Complex Formation in Ivanovo, Russia, 1998 (plenary talk).
149. Dong-Qing Wei, "Ab Initio MD and Its Application", Second International Conference on Frontiers of and Meeting of Chinese Physical 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", American Chemical Society National Las Vegas, September, 1997.
151. Dong-Qing Wei and D.R. Salahub, "Hydrated Proton Clusters: Structure, Spectroscopy and Ab Initio Dynamics", Research NH, USA,Aug 1996.
152. Dong-Qing Wei "Theory and Simulation of Strongly Interacting Dipolar Fluids: Ferroelectric Liquid Crystals, Ferrofluids and Electrorheological Fluids", First International Conference on Frontiers of Physics: Looking to the 21st 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", Second Canadian Computational Chemistry 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, Canadian Society for Chemistry Conference and 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", 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", 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 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", Second National Conference on Thermodynamics, Thermochemistry and September 1984, Wuhan, China.
162. Dong-Qing Wei, "Time Oscillation Study of a Two Molecule Three Intermediate Reaction", Fourth National Conference on Non-equilibrium Statistical Mechanics", October 1984, Guilin, China.
163. Dong-Qing Wei, "Markov Processes in Meteorology", on the Application of Statistical Physics on Meteorology", September 1983, Xinjiang, China.

Membership and Professional Affiliations

Fellow, The Royal Society of Chemistry(FRSC), since 2022;

Editor-in-Chief, -

Editor-in-Chief

Editor-in-Chief ational BioMedicine 3

Co-Editor (Bioinformatics),

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

Editorial Board: of Molecular Modeling and & Peptide of Atomic and Molecular Physics (In Chinese

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

Organizing Committee Member, Dec. 9-12, 2021, Houston, TX, USA.

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

Organizing Committee Member and Session Chair, IEEE International Conference on Bioinformatics and Biomedicine 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, Conference of Theory and Applications of Computational Chemistry 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, IEEE International Conference on Bioinformatics and Biomedicine November 18-21, 2019, San Diego, CA, USA.

Organizing Committee Member, IEEE International Conference on Bioinformatics and Biomedicine Dec 3-6, 2018, Madrid, Spain.

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

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

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

Organizing Committee Member, IEEE International Conference on Bioinformatics and Biomedicine November 17, 2017, Kansas City, Missouri, USA.

Organizing Committee Member, Conference on Proteomics (ICP-´ November 20-21,

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. Early Detection of Lung Cancer And Tuberculosis Using E-TRF-based Biosensors， China-Finland Intergovernmental Joint Funded Project, National Key Research Project, Project No. 2023YFE0199200, October 2023 September 2026, 4Million RMB, Project Leader.
2. Prediction of Drug-Target Interactions Using

10. Computer Aided Drug Design, First Class Course Building, Shanghai Jiaotong University, 2019.
11. Pharmacology Research and New Drug Development of Mangostin

29. 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.
30. 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.
31. Molecular Dynamics Simulation of Typical Explosives, National Key Lab. on Explosive Science and Technology, 2009-2011, Project Leader, Project No. KFJJ09-02.
32. Molecular Dynamics Simulation of Typical Explosives, National Key Lab. on Explosive Science and Technology, 2012-2014, Project Leader, Project No. KFJJ12-02.
33. Drug Discovery Technology Based on Effective Components and Multi-Targets, Ph.D. Research Funds, Ministry of Education, Project Leader, 2012-2014, project No.: 20120073110057.
34. Biophysics Joint Lab., Shanghai Bureau of Experts, 2012-2013, Project Leader.
35. Funding For International Journal of Third Phase, Shanghai Jiao Tong University, 2013-2014, Project Leader.
36. Publishing Funding for Simulation and Computer Aided Drug National Publishing Funds, 2012-2013, Project Leader.
37. Major Foreign High-Level Expert Funding, National Expert Bureau, 2011-2013, Project Leader.
38. Conference Grant for the International Conference on Computational and System Biology (ICCSB, 2009), Shanghai, China, Oct. 11-13, National Science Foundation.
39. Design and Screening of Leading Compounds for Anti-Alzheimer Disease, and Relevant Theoretical Studies, National Science Foundation, 2009-2011, project leader, project No 30870476.
40. Theoretical and Computational Method and its Application of Chemical Reactions in Complex Environments, National Science Foundation, 2008-2010, project leader, project No. 20773085.
41. National Comprehensive Technology Platforms For Innovative Drug R&D, as a PI, 2009-2010, Project No. 2009ZX9301-007.
42. 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.
43. Conference Grant for the IEEE Bioinformatics and Biomedical Engineering, Shanghai, China, May 16-18, National Science Foundation, project leader, 2008.
44. Funding for International Journals by funds from Jiao Tong University, project leader, 2008.
45. Study on the aggregation mechanism of amyloid fibrils, National Science Foundation, 2008-2011, PI, project No. 30770502.
46. Theoretical Studies of The HMX Explosives, Chinese Academy of Engineering Physics and also National Key Lab. on Explosives, 2007-2009, project leader.
47. 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.
48. 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.

49. Design, Screening, Synthesis and Optimization of Inhibitors Against SARS, The Tianjin Commission of Education, project leader, Project No. 20030001, 2004-2006.
50. 3-D Structure Determination Using Bioinformatics, The Tianjin Commission of Science and Technology, project leader, Project No. 023618211, 2002-2005.
51. Ab Initio Molecular Dynamics Simulation of Energetic Liquids, Chinese National Science Foundation, project leader, Project No. 10376024, 2004-2006.
52. 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. Nomination for The First-Class Award of Na Tm0 g0 G[(N)5(obe)9(l)] TJETQ EMC /P <</MCID 309>>

16. Nominated for the 10 Most Important Scientific Advancements 2010-2011, Ministry of Education.
17. Nominated for the Achievement in Asia Award (Robert T. Poe Prize)
18. Research Council UK for China Summer School Competition
19. Award from K.C.WONG EDUCATION FOUNDATION, Hong Kong for international conferences
20. Shanghai Mengminwei Award for 2009.
21. Shanghai Mengminwei Award for 2008.
22. 2012 Contributed the to the Chinese Science Bulletin.
23. The best paper award of 2006(the first time) by <Acta Pharmaceutica Sinica> for Inhibitor Screening Based on The Traditional Chinese Medicines Acta Pharmaceutica Sinica, 41(3), 241-246 (2006)(Figure was placed on the cover of the issue).
24. Shanghai Baiyulan Award for 2009.
25. Shanghai Baiyulan Award for 2006.
26. Shanghai Mengminwei Award for 2006.
27. 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

28. 1. The best thesis award for undergraduate students, Beijing University to Li Lin, July 2007.
29. 2. The Morgan Stanley Award administrated by the Shanghai Jiao Tong University to Li Lin, Oct. 2007.
30. 3. The national first prize of mathematics modeling to students Liang Jianyi and Shang Yuan, Nov. 2007.
31. 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.
32. 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.
33. The Qiushi graduate student awards to Lian Peng, The Jienengke 2nd prize for WangYing, The Jenengke 3rd Prize for Li Li, Oct. 2011.
34. 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.
35. Shanghai Jiao Tong University-AMD High Performance Computational Awards to YukunWang. 8, 2013.
36. 9. The Outstanding Ph.D. Student to Ruoxu Gu by the Shanghai Educational Commission, 2016.
37. The Outstanding Graduate Student awarded by the Shanghai Jiaotong University, Yanjing Wang Ph.D. student, Yanjing Wang, 2018.
38. The Outstanding Graduate Student awarded by the Shanghai Jiaotong University, Yanjing Wang Ph.D. student, Chengdong Li, 2019.
39. 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.
40. The National Graduate Student Award to Ph.D. student, Yanyi Chu, 2020.
41. The National Graduate Student Award to Ph.D. student, Yanyi Chu, 2021.

42. The Outstanding Graduate Student awarded by the city of Shanghai to Ph.D. student, Yanyi Chu, 2022.
43. Nomintion For Outstanding Ph.D. Thesis, Shanghai Jiaotong University, Yanyi Chu, 2022.
44. The Outstanding Undergraduate Student awarded by the city of Shanghai to

11. Databases of SNPs and enzymatic properties of CYP450 enzymes V1.0, 2010SR042161, 2010.08.18.
12. Database of drugs-targets and screening platform based on networks V1.0, 2010SR042163, 2010.08.18.
13. deMon Gui, V1.0, 2012SR090355.
14. Anti-cancer Vaccine Scanner (ACVA: precision based

Qiuying Dai	Shanghai Jiao Tong University	2018.9	Protein-Protein Interactions	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
Braden Stephens Keiser	Shanghai Jiao Tong University	2021.9	MD and enzyme	Master in progress

Students Graduated since 2005

Name	University	Date Graduated	Project	Status	Current Position
Ashma Sindhoo	Shanghai Jiao Tong University	2023.6	Cancer Informatics	Ph.D.	SZABIST University in Karachi, Pakistan as an Assistant Professor
Yanyi Chu	Shanghai Jiao Tong University	2022.7	Cancer Immunology	Ph.D.	Postdoc at Standford
Abbas Khan	Shanghai Jiao Tong University	2022.7	Covd-19 Drug and Infection Mechenism	Ph.D.	Spuer-postdoc at Shanghai Jiao Tong University
Juan Huang	Shanghai Jiao Tong University	2022.7	Cyp450 Molecular MD	Ph.D.	Researcher in Pharma. Company in Shanghai
Taimoor Khan	Shanghai Jiao Tong University	2021.11	Databases and human pathogenic viruses	Ph.D.	Postdoc Univ. of San Francisco
Wei Wang	Shanghai Jiao Tong University	2021.6	Statisitcal and AI models of mRNA and diseasea	Ph.D.	Hehuang Pharma
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
Yanjing Wang	Shanghai Jiao Tong University	2019.9-	Molecular Simulation, Drug Design	PhD	Lecturer at Shanghai Jiao Tong 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	Shanghai Jiao	2019.6	Membrane Permeation	Ph.D.	Shanghai University

Guan	Tong 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				

	Tong University		Human Cytochrome P450 and Protein-Chemical Interactions		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 -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
Muhammad Imran Sarwer	University Lahore as a foreign supervisor	2023.7	Molecular characterization of second-line drugs resistance mycobacterium tuberculosis clinical isolates	Ph.D.	Post-doc
Muhamma	University	2023.7	Whole genome	Ph.D.	Post-doc

d Zeeshan Anwar	Lahore as a foreign supervisor		sequencing and phylogenetic analysis of sars-cov-2 variants in Pakistani isolates		
Shifeng Jiang	Shanghai Jiao Tong University	2024.7	Vaccine design and AI	M.Sc.	Ph.D. in US
Haowei Huang	Qinghua Univ.	2023.7	Machine learning	M.Sc.	Ph.D. Qinghua
Shah Zeb Khan	Shanghai Jiao Tong University	2023.7	Vaccine design	M.Sc.	Back to Pakistan
Bowen Zhao	Shanghai Jiao Tong University	2023.7	Machine learning	M.Sc.	Ph.D. in McGill
Weizhi Chen	Shanghai Jiao Tong University	2023.7	MD simulation	M.Sc.	Company in Sh
Mingming Jiang	Shanghai Jiao Tong University	2023.7	Deep Learning	M.Sc.	Company in Sh
Jing Zhao	Shanghai Jiao Tong University	2023.7	Machine learning	M.Sc.	Ph.D. in McGill
Chujun Lv	Shanghai Jiao Tong University	2023.7	Machine learning	M.Sc.	Ph.D. in Swisland
Zhili Zhang	Shanghai Jiao Tong University	2018.9-	Personalized Drug	M.Sc.	Company in Sh
Yatong Liu	Shanghai Jiao Tong University	2018.9	Protein Interactions	M.Sc.	Company in Sh
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-	-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 Na ïve 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

			Virus B Proton Channel		
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 University	2009.7	Research on HIV-1 Protease Drug Resistance and Virtual screening for Possible Drug Candidates for Alzheimer's Disease.	M.Sc.	Ph.D in Rutgers University, USA
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.	Shenyang High School
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	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.	Tianjin High School
Shuqing Wang	Tianjin Normal University	2006.7	Cleavable Peptides of SARSCoV Mpro and Chemical Modification of Octapeptides	M.Sc.	Tianjin Medical University
Longhao Che Zhou	Shanghai Jiao Tong University	2023.7	Attention Network	B.S.	Ph.D. SJTU
Zhongyi Wang	Shanghai Jiao Tong University	2023.7	Machine Learning	B.S	Ph.D. Peking Univ.
Zilin Cai	Shanghai Jiao Tong University	2022.7	Machine Learning	B.S.	Ph.D. Qinghua Univ.
Lingfeng Zhang	University of Ottawa	2022.7	Machine Learning	B.S.	Graduate School
Hongfan Mu	University of Ottawa	2022.7	Machine Learning	B.S.	Graduate School
Zhongyi Wang	Shanghai Jiao Tong University	2022.7	Machine learning	B.S.	Ph.D. SJTU
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	Machine Leaning	B.Sc	HK Univ.
Tianhang Chen	Shanghai Jiao Tong University	2021.7			

Dai	Jiaotong University				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	Undergra duate	Ph.D. in US
Zhuofei Meng	Shanghai Jiao Tong University	2014.7-	MD Simulations	Undergra duate	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 Leaning	B.Sc	HK Univ.

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	2021-2023	AI cancer	Ph.D.	Post-doc
Muhammad Suleman	Shanghai Jiaotong University	2019-2022	Covid-19	Ph.D.	Post-doc
Ying Sun	Shanghai Jiaotong University	2023-	Big data	Ph.D.	Post-doc
Yifan Jin	Shanghai Jiaotong University	2021-2023	Vaccine	Ph.D.	Post-doc
Jiayi Li	Shanghai Jiaotong University	2023-	MD and catalysis	Ph.D.	Post-doc
Elise Dumont	Institut de Chimie de Nice ICN, UMR CNRS	2022-	QM/MM	Ph.D.	Visiting Professor