Curriculum Vitae

Meng Cui, Ph.D.

PERSONAL INFORMATION

Name: Meng Cui
Title: Research Associate Professor
Institution Name: Department of Pharmaceutical Sciences, School of Pharmacy, Northeastern University
Address: 805 Columbus Ave, Boston, MA 02120
Email: m.cui@northeastern.edu

Primary Departmental Program Area: Molecular Biophysics
Areas of expertise and interest:

- Structure and function of membrane proteins, such as GPCRs and Ion channels
- Ligand-protein, and protein-protein interactions
- Structure-based drug discovery

EDUCATION

Sept. 1994-July 1999, Doctor of Science (Physical Chemistry)
Institute of Theoretical Chemistry, Jilin University, PR China
Sept. 1990-July 1994, Bachelor of Science (Organic Chemistry)
Dept. of Chemistry, Heilongjiang University, PR China

PROFESSIONAL EXPERIENCE

Feb 2017- Research Associate Professor, Department of Pharmaceutical Sciences, Northeastern University, Boston, MA, USA
July 2014- Feb 2017 Principle Scientist, Eurofins Lancaster Laboratories, Richmond, VA, USA
July 2014-Jun 2016 Adjunct professor, Department of Physiology & Biophysics, Virginia Commonwealth University, Richmond, VA, USA
Jun 2008- Jun 2014 Research Assistant Professor, Department of Physiology & Biophysics, Virginia Commonwealth University, Richmond, Virginia, USA
Nov 2004- Jun 2008 Instructor, Department of Physiology & Biophysics, Mount Sinai School of Medicine, New York, USA
Sep 2003-Dec 2004 Postdoc, Biophysics, Department of Molecular Physiology & Biophysics, Mount Sinai School of Medicine, New York, USA
Sep 2001-Aug 2003 Postdoc, Computational Biology, Department of Biology and Biochemistry, University of Houston, USA
Sep 1999-Aug 2001 Postdoc, Computational Biology, State Key Laboratory of Drug Research, Shanghai Institute of Meteria Medica, Chinese Academy of Sciences, P. R. China

OTHER EXPERIENCE

Journal reviewer: Journal of Computer-Aided Molecular Design
Current Computer-Aided Drug Design

PLoS Computational Biology
PLoS One
Proteins: Structure, Function, and Bioinformatics
Journal of Chemical Theory and Computation
Biochimica et Biophysica Acta
Langmuir
Journal of Molecular Graphic and Modeling
Biopolymers
BMC Bioinformatics
Journal of Chemical information and Modeling
Journal of Biology Chemistry
Biophysical Journal
Molecular Informatics
Chemical Biology & Drug Design
Food & Function
Molecular BioSystems

Journal guest editor: Current Pharmaceutical Biotechnology, 2014

Grant reviewer: Center for Scientific Review Special Emphasis Panel
ZRG1 ETTN-H (51) June 09, 2009 – June 15, 2009
Center for Scientific Review Special Emphasis Panel
ZRG1 ETTN-H (51)R Mar 22, 2010 – Mar 23, 2010
NIH, Biophysics of Neural Systems Study Section, Feb. 17-18, 2011
NIH, Eunice Kennedy Shriver National Institute of Child Health & Human Development (NICHD) Dec. 2, 2013
Biotechnology and Biological Sciences Research Council(BBSRC), UK, Apr. 9, 2015

MEMBERSHIP

1. New York Academy of Science, 2005-2006
2. Association for Chemoreception Science, 2005-2006
3. American Chemical Society, 2003-
4. Biophysical Society, 2005-
5. Society for Neuroscience, 2011-
6. American Heart Association, 2011-

GRANTS

1. China Postdoctoral Grant (PI), China Postdoctoral Science Foundation, 28th, 2000.
2. Shanghai Postdoctoral Grant (PI), Shanghai Science & Technology Committee, 2000.
3. Pittsburgh Supercomputing Center (PSC) grant (PI, MCB060020), 2006-2007.
4. Teragrid Supercomputing grant (PI, TG-MCB070095T), 2007-2008.
5. NIH Small Research Grant (PI, R03: DC007721), 2005-2008.
   Mechanism of Agonism-Antagonism of Sweet Taste Receptors
6. NIH R21 Research Grant (PI, R21DC008996), 2008-2011.
   Modeling Sweet Protein-Receptor Interactions

7. NIH R21 Research Grant, supplement (PI, R21DC008996-01A2S1), 2009-2011, Modeling Sweet Protein-Receptor Interactions
8. NIH/Shared Instrumentation Grant Program (S10) (PI, S10RR027411), 2010-2013, High Performance Computing Cluster for Biomedical Research at VCU

RESEARCH INTRESTS

My research focuses on understanding the relationship between structure and function of membrane proteins, such as G Protein-Coupled Receptors (GPCRs) and Ion channels. In this collaborative effort we utilize computational modeling techniques, molecular mutagenesis and functional expression of the receptors and channels to understand the signal-recognition and transduction mechanism of these important macromolecules. By means of computational and experimental approaches, we seek to understand how ligands or proteins interact and activate their targeting receptors or ion channels. Molecular Dynamics (MD) simulations based on all-atomic are being used to understand the ligand induced activation mechanism of ion channels. We are also developing computational approaches for loop modeling, flexible protein-ligand and protein-protein docking to achieve these goals.

PUBLICATIONS

68. Marmolejo-Murillo LG, Aréchiga-Figueroa IA, **Cui M**, Moreno-Galindo EG, Navarro-Polanco RA, Sánchez-Chapula JA, Ferrer T, Rodríguez Menchaca AA.Inhibition of Kir4. 1 potassium channels by quinacrine. ***Brain Res***. 2017, 1663, 87-94

67. Marmolejo-Murillo LG, Aréchiga-Figueroa IA, Moreno-Galindo EG, Navarro-Polanco RA, Rodríguez-Menchaca AA, **Cui M**, Sánchez-Chapula JA, Ferrer T. Chloroquine blocks the Kir4.1 channels by an open-pore blocking mechanism. ***Eur J Pharmacol.*** 2017, 800, 40-47.

66. Tobelaim WS, Dvir M, Lebel G, **Cui M**, Buki T, Peretz A, Marom M, Haitin Y, Logothetis DE, Hirsch JA, Attali B. Competition of calcified calmodulin N lobe and PIP2 to an LQT mutation site in Kv7.1 channel. ***Proc Natl Acad Sci U S A.*** 2017 Jan 31;114(5): E869-E878.

65. XY Meng, S Liu, **M Cui**, R Zhou, DE Logothetis. The Molecular Mechanism of Opening the Helix Bundle Crossing (HBC) Gate of a Kir Channel. ***Scientific Reports*** 2016, 6

64. JL Moreno, P Miranda-Azpiazu, A García-Bea, J Younkin, **M Cui**, Alexey Kozlenkov, Ariel Ben-Ezra, Georgios Voloudakis, Amanda K Fakira, Lia Baki, Yongchao Ge, Anastasios Georgakopoulos, José A Morón, Graeme Milligan, Juan F López-Giménez, Nikolaos K Robakis, Diomedes E Logothetis, J Javier Meana, Javier González-Maeso. Allosteric signaling through an mGlu2 and 5-HT2A heteromeric receptor complex and its potential contribution to schizophrenia. ***Sci. Signal.*** 2016, 9 (410), ra5-ra5

63. DE Logothetis, R Mahajan, SK Adney, J Ha, T Kawano, XY Meng, **M Cui**. Chapter One-Unifying Mechanism of Controlling Kir3 Channel Activity by G Proteins and Phosphoinositides. ***International review of neurobiology*** 2015, 123, 1-26

62. EL Maillet*, **M Cui***, P Jiang, M Mezei, E Hecht, J Quijada, RF Margolskee, R. Osman, M. Max Characterization of the binding site of aspartame in the human sweet taste receptor. ***Chemical senses*** 2015, 40 (8), 577-586

61. M Zhang, XY Meng, J Zhang, **M Cui**, DE Logothetis. Molecular overlap in the regulation of SK channels by small molecules and phosphoinositides. ***Science advances*** 2015, 1 (6), e1500008

60. Q. Y. Tang, T. Larry, K. Hendra, E. Yamamoto, J. Bell, **M. Cui**, D. Logothetis, L. M. Boland. Nature's Mutations Evolved a High Affinity PIP2 Binding Site In Vertebrate Inwardly Rectifying Potassium Channels. ***J Biol Chem.*** *2015, 290 (27), 16517-16529*

59. D. E. Logothetis, V. I. Petrou, M. Zhang, R. Mahajan, X.-Y. Meng, S. K. Adney, **M. Cui**, and L. Baki. PHOSPHOINOSITIDE CONTROL OF MEMBRANE PROTEIN FUNCTION: A Frontier Led by Studies on Ion Channels. ***Annu. Rev. Physiol.*** 2015. 77

58. C. Hatcher-Solis, M. Fribourg, K. Spyridaki, J. Younkin, A. Ellaithy, G. Xiang, G. Liapakis, J. Gonzalez-Maeso, H. Zhang, **M. Cui**, and D. E. Logothetis. G Protein-Coupled Receptor Signaling to Kir channels in Xenopus Oocytes, ***Current Pharmaceutical Biotechnology***, 2014, 15 (10), 987-995

57. **M. Cui**, G. Qin, K. Yu, M.S. Bowers, M. Zhang. Targeting the Small- and Intermediate-Conductance Ca2+-Activated Potassium Channels: The Drug-Binding Pocket at the Channel/Calmodulin Interface. ***Neurosignals,*** 2014, 22 (2), 65-78

56. X.-Y. Meng, M. Mezei and **M. Cui***. Computational Approaches for Modeling GPCR Dimerization, ***Current Pharmaceutical Biotechnology***, 2014, 15 (10), 996-1006

55. Q. Y. Tang, Z. Zhang, X. Y. Meng, **M. Cui**, D. E. Logothetis. Structural determinants of phosphatidylinositol 4,5-bisphosphate (PIP2) regulation of BK channel activity through the RCK1 Ca2+ coordination site. ***J Biol Chem.*** 2014 Jul 4;289(27):18860-72.

54. M. Zhang, X.-Y. Meng, **M. Cui**, J. M. Pascal, D. E. Logothetis, J. F. Zhang. Selective phosphorylation modulates the PIP2 sensitivity of the CaM-SK channel complex. ***Nat Chem Biol.*** 2014 Sep;10(9):753-9.

53. Y. Xu, Y.-H. Wang, X.-Y. Meng, M. Zhang, M. Jiang, **M. Cui**, G.-N. Tseng. Building KCNQ1/KCNE1 docking models and probing their interactions by molecular dynamics simulations. ***Biophys J*** 2013;105:2461-2473 (see related New & Notable)

52. Moretti R, Fleishman SJ, Agius R, Torchala M, Bates PA, Kastritis PL, Rodrigues JP, Trellet M, Bonvin AM, **Cui M**, Rooman M, Gillis D, Dehouck Y, Moal I, Romero-Durana M, Perez-Cano L, Pallara C, Jimenez B, Fernandez-Recio J, Flores S, Pacella M, Praneeth Kilambi K, Gray JJ, Popov P, Grudinin S, Esquivel-Rodríguez J, Kihara D, Zhao N, Korkin D, Zhu X, Demerdash ON, Mitchell JC, Kanamori E, Tsuchiya Y, Nakamura H, Lee H, Park H, Seok C, Sarmiento J, Liang S, Teraguchi S, Standley DM, Shimoyama H, Terashi G, Takeda-Shitaka M, Iwadate M, Umeyama H, Beglov D, Hall DR, Kozakov D, Vajda S, Pierce BG, Hwang H, Vreven T, Weng Z, Huang Y, Li H, Yang X, Ji X, Liu S, Xiao Y, Zacharias M, Qin S, Zhou HX, Huang SY, Zou X, Velankar S, Janin J, Wodak SJ, Baker D., Community-wide Evaluation of Methods for Predicting the Effect of Mutations on Protein-Protein Interactions. ***Proteins.*** *2013 Nov;81(11):1980-7.*

51. M. Dewis, T. Phan, X. Meng, **M. Cui**, S. Mummalaneni, M. Rhyu, J. DeSimone, V. Lyall, N-geranylcyclopropylcarboximide (NGCC) Modulates Salty And Umami Taste In Humans And Animal Models, ***Journal of Neurophysiology*** 2013 Feb;109(4):1078-90

50. Y. Wang, M. Zhang, Y. Xu, M. Jiang, D. P. Zankov, C. Tian, **M. Cui**, and G. N. Tseng, Probing the structural basis for differential KCNQ1 modulation by KCNE1 and KCNE2, ***J Gen Physiol*** 2012;140:653-669

49. H. An, S. Lü, J. Li, X. Meng, Y. Zhan, **M. Cui**, M. Long, H. Zhang, D. E. Logothetis, Control of Kir2 Channel Gating Transitions of the Cytosolic Gate by Distinct Regulatory Loops. ***J Biol***

***Chem** 2012 doi: 10.1074/jbc.M112.418640 jbc.M112.418640*

48. B. Liu, M. Ha, XY Meng, M. Khaleduzzaman, Z. Zhang, X. Li, **M. Cui***. Functional characterization of the heterodimeric sweet taste receptor T1R2 and T1R3 from a New World monkey species (squirrel monkey) and its response to sweet-tasting proteins. ***Biochem Biophys Res Commun.*** 2012, 427(2):431-7 *(*: corresponding author)*

47. A. A. Rodriguez-Menchaca, S. K. Adney, Q. Y. Tang, X. Meng, A. Rosenhouse-Dantsker, **M. Cui**, and D. E. Logothetis, PIP_2 Controls Voltage Sensor Movement and Pore Opening of Kv Channels through the S4-S5 Linker. ***Proceedings of the National Academy of Sciences***, 2012, 109(36):E2399-408.

46. X. Y. Meng, H. X. Zhang, D. E. Logothetis***,** and **M. Cui***, The molecular mechanism by which PIP_2 opens the intracellular G-loop gate of a Kir3.1 channel. ***Biophysical Journal*** 2012, May (102) 2049-2059. *(*: corresponding author)*

45. X. Y. Meng, Y. Xu, H. X. Zhang, M. Mezei, **M. Cui***, Protein-Protein Docking using a Brownian Dynamics Simulations Approach, ***Journal of Biomedicine and Biotechnology*** 2012, Article ID 121034 *(*: corresponding author)*

44. B. Liu, M. Ha, X. Y. Meng, T. Kaur, M. Khaleduzzaman, Z. Zhang, P. Jiang, X. Li, **M. Cui***, Molecular Mechanism of Species-dependent Sweet Taste toward Artificial Sweeteners, ***Journal of Neuroscience***, 2011 Jul 27;31(30):11070-6. *(*: corresponding author)*

43. X. Y. Meng, H. X. Zhang, M. Mezei, **M. Cui***, Molecular Docking: A powerful approach for structure-based drug discovery, ***Current Computer-Aided Drug Design*** *2011; Jun 1;7(2):146-57. (*: corresponding author)*

42. M. Cui*, M. Mezei*, and R. Osman, Prediction of protein loop structures using a local move Monte Carlo approach and a grid-based force field, ***Protein Eng. Des. Sel.***, *2008* (21), 729-735. *(*: corresponding author)*

41. M. Cui*, M. Mezei, R. Osman*, Modeling Transmembrane Dimerization by Brownian Dynamics Simulations. ***J Comput Aided Mol Des*** *2008;* Aug; 22(8):553-61*(*: corresponding author)*

40. M. Cui, P. Jiang, E. Maillet, M. Max, R. Margolskee, R. Osman, MODELS OF SWEET TASTE RECEPTORS PROVIDE INSIGHTS INTO FUNCTION. In: Sweetness and Sweeteners: Biology, Chemistry and Psychophysics. ***ACS Symposium Series*** 979; D.K. Weerasinghe and G.E. DuBois, Eds..; American Chemical Society, Washington, DC, *2008*, p117-132.

39. P. Jiang, E. Maillet, **M. Cui**, R. Osman M. Max, R. Margolskee, MAKING SENSE OF THE SWEET TASTE RECEPTOR. MODELS OF SWEET TASTE RECEPTORS PROVIDE INSIGHTS INTO FUNCTION. In: Sweetness and Sweeteners: Biology, Chemistry and Psychophysics. ***ACS Symposium Series*** 979; D.K. Weerasinghe and G.E. DuBois, Eds..; American Chemical Society, Washington, DC, *2008*, p48-64.

38. M. Cui, P. Jiang, E. Maillet, M. Max, R. Margolskee, R. Osman. The Heterodimeric Sweet Taste Receptor has Multiple Potential Ligand Binding Sites. ***Curr Pharm Des. 2006;*** 12(35): 4591-600.

37. P. Jiang, **M. Cui**, B. Zhao, LA Snyder, LM Benard, R Osman, M Max, RF Margolskee. Identification of the cyclamate interaction site within the transmembrane domain of the human sweet taste receptor subunit T1R3. ***J Biol Chem. 2005*** Oct 7;280(40):34296-305.

36. P. Jiang, **M. Cui**, B. Zhao, Z. Liu, L. A. Snyder, L. M. Benard, R. Osman, R.F. Margolskee, M. Max. Lactisole interacts with the transmembrane domains of human T1R3 to inhibit sweet taste**.** ***J Biol Chem. 2005*** Apr 15;280(15):15238-46.

35. J. Deng, K. W. Lee, T. Sanchez, **M. Cui**, N. Neamati, J. M. Briggs. Dynamic Receptor-Based

Pharmacophore Model Development and Its Application in Designing Novel HIV-1 Integrase Inhibitors**. *J Med Chem. 2005*** Mar 10;48(5):1496-505.

34. P. Jiang, **M. Cui**, Q. Ji, L. Snyder, Z. Lui, L. Benard, R.F. Margolskee, R. Osman and M. Max Molecular Mechanisms of Sweet Recptor Function. ***Chem Senses. 2005*** Jan;30 Suppl 1:i17-i18.

33. X. Huang, H. Liu, **M. Cui**, W. Fu, K. Chen, X. Luo, J. Shen, H. Jiang. Simulating the interactions of toxins with K+ channels. ***Curr Pharm Des. 2004;*** 10(9):1057-67.

32. B. Tan, M. C. Lee, **M. Cui**, T. Liu, Z. Z. Chen, Y. M. Li, Y. Ju, Y. F. Zhao, K. Chen, H. Jiang. A common intermediate for prebiotic synthesis of proteins and nucleosides: a density functional theory (DFT) study on the formation of penta-coordinate phosphorus carboxylic-phosphoric mixed anhydride from N-phosphoryl amino acids. ***Journal of Molecular Structure:*** **THEOCHEM** ***2004***, 672: 51-60.

31. X. Huang, J. Shen, **M. Cui**, L. Shen, X. Luo, K. Ling, G. Pei, H. Jiang, K. Chen. Molecular Dynamics Simulations on SDF-1alpha: Binding with CXCR4 Receptor. ***Biophys J. 2003,*** 84(1):171-84.

30. M. Cui, X. Q. Huang, X. Luo, J. M. Briggs, R. Y. Ji, K. X. Chen, J. H. Shen, H. L. Jiang. Molecular Docking and 3D-QSAR Studies on Gag Peptide Analog Inhibitors Interacting with Human Cyclophilin A. ***J. Med. Chem. 2002***, 21;45(24):5249-59

29. M. Cui, J. H. Shen, J. M. Briggs, W. Fu, J. Wu, Y. Zhang, X. Luo, Z. Chi, R. Y. Ji, H. L. Jiang, K. X. Chen. Brownian Dynamics Simulations of the Recognition of the Scorpion Toxin P05 with the Small-conductance Calcium-activated Potassium Channels. ***J. Mol. Biol. 2002***, *318*, 417-428

28. M. Cui, W. Adam, J. H. Shen, X. Luo, X. Tan, K. X. Chen, R. Y. Ji, H. L. Jiang. A Density-Functional Study of the Mechanism for the Diastereoselective Epoxidation of Chiral Allylic Alcohols by the Titanium Peroxy Complexes. ***J. Org. Chem. 2002,*** *67*, 1427-1435

27. W. Fu, **M. Cui**, J. M. Briggs, X. Q. Huang, B. Xiong, Y. Zhang, X. Luo, J. H. Shen, R. Y. Ji, H. L. Jiang, K. X. Chen. Brownian Dynamics Simulations of Interaction Between Scorpion Toxin Maurotoxin and Voltage-gated Potassium Ion Channel. ***Biophys J.*** **2002**, 83(5):2370-85

26. M. Cui, J. H. Shen, J. M. Briggs, X. J. Tan, H. L. Jiang, K. X. Chen, R. Y. Ji. Brownian Dynamics Simulations of Interaction Between Scorpion Toxin Lq2 and Potassium Ion Channel. ***Biophys J. 2001***, 80, 1659-1669

25. X. J. Tan, W. L. Zhu, **M. Cui**, X. M. Luo, J. D. Gu, I. Silman, J. L. Sussman, H. L. Jiang, R. Y. Ji, K. X. Chen. Noncovalent interaction or chemical bonding between alkaline earth cations and benzene? A quantum chemistry study suing MP2 and density-functional theory methods. ***Chem. Phys. Lett. 2001***, 113-122

24. M. Cui, J. K. Feng, S. F. Wang, C. C. Sun, J. B. Liu, Z. Gao, F. A. Kong. Theoretical studies of lead-sulfur binary Pb5S4+ clusters. ***Chem. J. Chinese Univ.*** *2000*, 21 (2): 260-262

23. M. Cui, J. K. Feng, S. F. Wang, M. F. Ge, C. Sun. *Ab initio* studies on $Ti_8C_{12}H_4(T_d)$ and $Ti_8C_{12}H_8(T_d)$ clusters. ***Chem. J. Chinese Univ. 2000***, 21(6), 908-11

22. J.K. Feng, W. Fu, **M. Cui**, Z. M. Su, A. M. Ren. Calculations on the Electronic Structure and Nonlinear Second-Order Susceptibility of C_{60} Pyrrolidine/Ferrocene Based Donor-Bridge-Acceptor Dyads. ***Acta Chimica Sinica. 2000***, 58, 1112-9

21. W. Fu, J. K. Feng, A. M. Ren, **M. Cui**, H. W. Jin. Theoretical studies of molecules with nonlinear optical third-order susceptibilities on pull-push multi-cycle electro-optical polymer intermediates including thiophene-ring. ***Chem. J. Chinese Univ. 2000***, 21(5), 771-775

20. S. F. Wang, J. K. Feng, K. Q. Yu, **M. Cui**, A. Ren, C. Sun, P. Liu, Z. Gao, F. Kong. DFT studies of structures and vibrational spectra of silicon-sulfur clusters $(SiS_2)_n^+$ (n=1-5). ***J.***

Molecular structure (Theochem). 2000, 499, 241-255

19. S. F. Wang, J. K. Feng, **M. Cui**, C. C. Sun, P. Liu, Z. Gao, F. A. Kong. Quantum chemical study of silicon-sulfur clusters(SiS2)(n)(+)(n=1-3). ***Chem. J. Chinese Univ. 2000***, 21 (2): 255-259

18. W. Fu, J. K. Feng, A. M. Ren, **M. Cui**, H. W. Jin, J. H. Wang, Y. Q. Shen. Studes on the device of molecules with nonlinear optical second-order susceptibilities on novel pull-push dicycle electro-optical polymer intermediates including thiophene-ring. ***J. Mol. Sci. 2000***, 16, 5-11

17. W. Fu, J. K. Feng, K. Q. Yu, A. M. Ren, **M. Cui**, Y. Li, C. Sun. Theoretical study on second-order nonlinear optical properties of unsymmetric bis (phenyethynyl) benzene series derivatives. ***Chinese J. Chem. 2000***, 18(2), 175-81

16. **M. Cui**, J. K. Feng, H. X. Zhang, M. F. Ge, C. Sun, J. P. Zhang. Dependence of multiplicity on conformation: ground states of o-, m- and p-phenylenediamine dications. ***Synth. Met. 1999***, 100, 261-8

15. **M. Cui**, H. Zhang, M. F. Ge, J. K. Feng, W. Tian, C. Sun. *Ab initio* studies of C_{40}, C_{40}^+, $Nb@C_{40}^+$, NbC_{59}^+, $Nb@C_{40}H_4^+$. ***Chem. Phy. Lett. 1999***, 309, 344-50

14. **M. Cui**, M. F. Ge, J. K. Feng, H. Zhang, W. Tian, C. Sun. *An ab initio* study on Silicon-doped carbon clusters. ***J. Molecular structure (Theochem). 1999***, 492, 241-56

13. **M. Cui**, J. K. Feng, M. F. Ge, S. F. Wang, C. Sun, Z. Gao, F. A. Kong. *Ab initio* study of silver-sulfur binary $[Ag(Ag_2S)_n]^+$ (n=1,2) clusters. ***Chem. J. Chinese Univ. 1999***, 20(3), 436-9

12. **M. Cui**, J. K. Feng, M. F. Ge, S. F. Wang, X. R. Huang, C. Sun, P. Liu, F. A. Kong. *Ab initio* study of silver-sulfur binary $[Ag(Ag_2S)_n]^+$ (n=3,4) clusters. ***Acta Chimica Sinica****. 1999*, 57, 672-9

11. **M. Cui**, J. K. Feng, M. F. Ge, S. F. Wang, C. Sun, J. B. Liu, Z. Gao, F. A. Kong. *Ab initio* studies of lead-sulfur binary $Pb_nS_{n-1}^+$(n=2~4) clusters. ***Acta Chimica Sinica****. 1999*, 57, 1062-7

10. **M. Cui**, J. K. Feng, S. F. Wang, M. F. Ge, W. Tian, C. Sun. *Ab initio* studies of C_nSi(n=35,36)clusters. ***J. Molecular Science 1999***, 15(4), 189

9. S. F. Wang, J. K. Feng, **M. Cui**, M. F. Ge, C. Sun, Z. Gao, F. A. Kong. Geometry and Stability of Vanadium-sulfide Clusters $V_2S_2^+$ and $V_3S_4^+$. ***Chem. J. Chinese Univ. 1999***, 20(9), 1447-51

8. M. F. Ge, J. K. Feng, **M. Cui**, S. F. Wang, W. Tian. Theoretical studies of various possible structure of C_nSi(n=28,29). ***Acta Chimica Sinica****. 1999*, 57, 645-52

7. M. F. Ge, J. K. Feng, **M. Cui**, S. F. Wang, W. Tian, C. Sun. *Ab initio* studies of various possible structures of C_nSi(n=49,50). ***Chem. J. Chinese Univ. 1999***, 20(5), 788-93

6. M. F. Ge, J. K. Feng, **M. Cui**, W. Tian, A. Ren, X. Y. Sun, C. Sun. Theoretical studies on the structure and vibrational spectrum of $N@C_{60}$. ***Chem. J. Chinese Univ. 1999***, 19(3), 458-60

5. W. Fu, J. K. Feng, A. M. Ren, **M. Cui**, X. Y. Sun, Y. X. Li. A ZINDO-SOS Study on nonlinear Second-order optical properties of unsymmetriec Bis(phenylethynyl) benzenes series derivatives. ***Acta Chimica Sinica. 1999***, 57, 1075-80

4. W. Fu, J. K. Feng, A. M. Ren, **M. Cui**, X. Y. Sun, Y. X. Li. A Theoretical Studies on nonlinear Second-order optical properties of p-Nitrobis (phenylethynyl) benzenes series derivatives. ***Chem. J. Chinese Univ. 1999***, 20(9), 1424-28

3. S. F. Wang, J. K. Feng, **M. Cui,** C. Sun, Z. Gao, F. A. Kong. Geometry and Stability of Cobalt-Sulfide Clusters $Co_nS_{n-1}^+$(n=2,3). ***Chem. J. Chinese Univ. 1999***, 20(12), 1931-5

2. J. N. Feng, **M. Cui**, X. R. Huang, P. Otto, F. L. Gu. Calculated properties of cationic phosphorus clustersP_{2n+1}^+ with n=3,4,5 and 6. ***J. Molecular Structure (Theochem). 1998***, 425, 201-6

1. M. F. Ge, J. K. Feng, **M. Cui**, S. F. Wang, W. Q. Tian, X. R. Huang, Z. R. Li. Quantum

chemical study of C-40,C-40(+),Nb@ C-40(+), NbC39+, Nb@ C40H4+ . ***Acta Chimica Sinica. 1998***, 56 (11): 1063-1069