基本信息

陈世稆	
教授，博士生导师	
shlchen@bit.edu.cn	
化学与化工学院/化学系/理论与计算化学研究所	

教育背景

2005/11 – 2009/02	瑞典皇家工学院，生物技术学院，“生物技术”博士
2004/09 – 2008/01	北京师范大学，化学学院，“物理化学”博士
2001/09 – 2004/07	北京师范大学，化学系，“分析化学”硕士
1997/09 – 2001/07	北京师范大学，化学系，“化学教育”学士

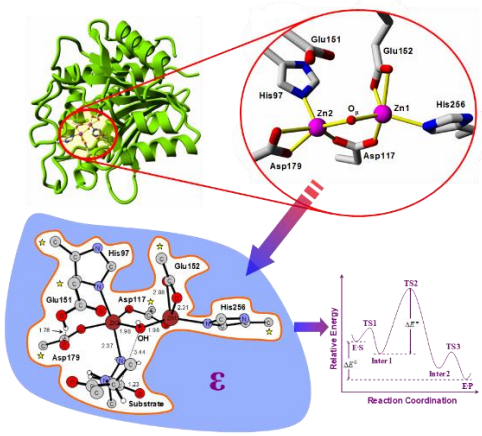
工作履历

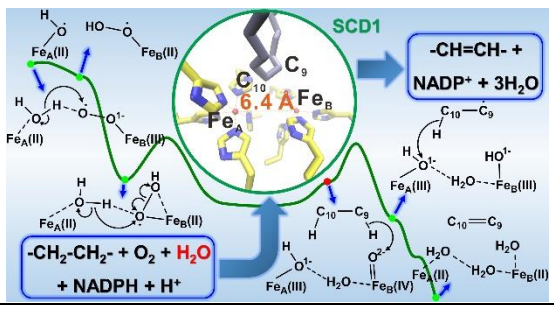
2012/07 – 至今	北京理工大学，化学学院，教授
2010/10 – 2012/07	北京理工大学，化学学院，副教授
2009/04 – 2010/09	瑞典斯得哥尔摩大学，物理系，博士后

研究方向

生物酶与均相催化反应机理的理论研究

运用理论化学手段，主要是密度泛函理论（DFT）方法，研究各种金属酶的催化反应机理。研究策略（下左）与结果示例（下右）如下：





研究对象包括多种过渡金属酶，成果示例如下：

Fe

ACS Catalysis 2019, 9, 4345
ChemPhysChem 2020, 21, 385
PCCP 2018, 20, 26500
J. Catalysis 2018, 360, 1
J. Catalysis 2017, 348, 40
Dalton Trans. 2016, 45, 2517
Dalton Trans. 2014, 43, 973

Ni

JACS 2009, 131, 9912
Chem. Eur. J. 2017, 23, 7545
Chem. Eur. J. 2012, 18, 6309
PCCP 2014, 16, 14029

Zn

J. Inorg. Biochem. 2018, 185, 71
J. Chem. Theory Comput. 2015, 11, 2525
ChemPhysChem 2014, 15, 2321
J. Inorg. Biochem. 2012, 111, 70
J. Inorg. Biochem. 2009, 103, 274
Biochemistry 2008, 47, 9497
J. Phys. Chem. B 2008, 112, 2494
Theor. Chem. Account 2008, 120, 515
J. Phys. Chem. B 2007, 111, 1253

W

Dalton Trans. 2019, 48, 5683

Co

JPC Letters 2020, 11, 6812
ACS Catalysis 2015, 5, 7350
J. Phys. Chem. B 2011, 115, 4066
J. Chem. Theory Comput. 2010, 6, 2040

Mg

ChemBioChem 2020, 21, 385
ChemPhysChem 2014, 15, 2321

Non-metal

J. Org. Chem. 2016, 81, 9289

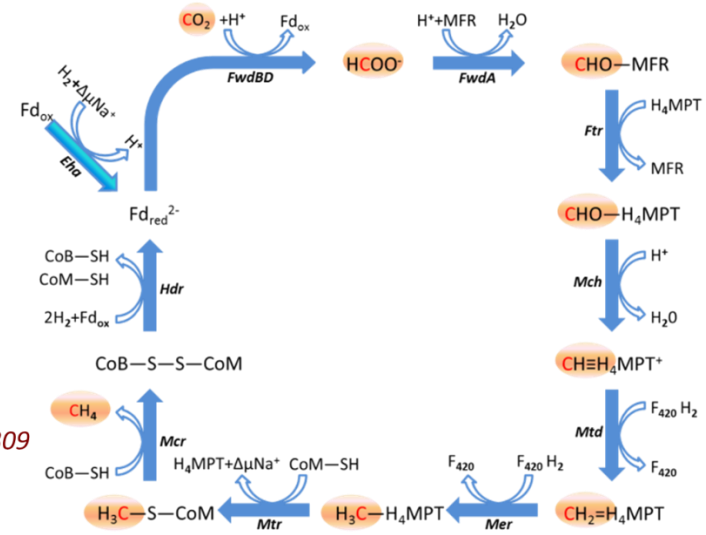
Ni Review

Per Siegbahn, Shi-Lu Chen, Rong-Zhen Liao, Inorganics, 2019, 7, 95

研究兴趣主要在各类特殊生境微生物代谢途径相关酶催化机理上，如，嗜热甲烷生成古菌代谢途径：

Methanogens: $CO_2 + 4\ H_2 \rightarrow CH_4 + 2H_2O$

J. Inorg. Biochem. 2018, 185, 71



JACS, 2009, 131, 9912
Chem. Eur. J., 2012, 18, 6309
PCCP, 2014, 16, 14029

再如，高氯酸盐还原菌代谢途径：

Perchlorate-reducing:

$$ClO_4^- \xrightarrow{Pcr} ClO_3^- \xrightarrow{Pcr} ClO_2^- \xrightarrow{Cld} Cl^- + O_2$$

Dalton Trans., 2019, 48, 5683

J. Catalysis, 2017, 348, 40
Dalton Trans., 2014, 43, 973

荣誉奖励

1.	国家留学基金管理委员会颁发的“2008 年度国家优秀自费留学生奖”
2.	北京理工大学 2010 年度“优秀青年教师”奖
3.	入选 2015 年度北京市科技新星计划

承担项目

1.	国家自然科学基金委员会，面上项目，21673019，硫微生物排放中酶催化反应机理的理论研究，2017-01 至 2020-12，主持
2.	国家自然科学基金委员会，面上项目，21373027，可用于太阳-化学能转化的生物酶及仿生体系催化反应机理的理论研究，2014-01 至 2017-12，主持。
3.	国家自然科学基金委员会，青年科学基金项目，21103010，含镍金属酶催化反应机理的理论研究，2012-01 至 2014-12，主持。

研究成果

主持国家自然科学基金项目 3 项；参与科技部 973 项目课题 1 项。入选 2015 年北京市科技新星计划。迄今发表 SCI 论文 60 余篇。

代表性论文

1	**Shi-Lu Chen*** and Per E. M. Siegbahn*, Insights into the Chemical Reactivity in Acetyl-CoA Synthase, ***Inorg. Chem.,* 2020,** DOI: 10.1021/acs.inorgchem.0c02139.
2	Shuo-Qi Sun and **Shi-Lu Chen***, An Unprecedented Ring-Contraction Mechanism in Cobalamin-Dependent Radical S-Adenosylmethionine Enzymes, ***J. Phys. Chem. Letters,* 2020,** 11, 6812-6818.
3	Haishan Yu, Ying Wang, Xijun Wang, Jinxiao Zhang, Sheng Ye, Yan Huang, Yi Luo, Edward Sharman*, **Shilu Chen***, Jun Jiang*, Using Machine Learning to Predict the Dissociation Energy of Organic Carbonyls, ***J. Phys. Chem. A,* 2020,** 124, 19, 3844–3850.
4	Ji-Fan Yan and **Shi-Lu Chen***, How To Produce Methane Precursor in the Upper Ocean by An Untypical Non-Heme Fe-Dependent Methylphosphonate Synthase?, ***ChemPhysChem,* 2020,** 21, 385–396.
5	Ming-Jia Yu and **Shi-Lu Chen***, Mechanism and Inhibitor Exploration with Binuclear Mg Ketol-Acid Reductoisomerase: Targeting the Biosynthetic Pathway of Branched-Chain Amino Acids, ***ChemBioChem,* 2020,** 21, 381–391.
6	Shan-Qing Peng, Butian Zhang, Wenhao Fan, Shuifeng Wang, Zhi-Hao Zhang, Yan Liu, **Shi-Lu Chen***, and Mu-Hua Huang, Facile synthesis of a porous polynorbornene with an azobenzene subunit: selective adsorption of 4-nitrophenol over 4-aminophenol in water, ***Polymer Chemistry,* 2020,** DOI: 10.1039/d0py00994f.

7	Yong-Chao Zheng, Jing-Xuan Su, He Zheng, Sheng-Song Li, Chong-Lin Zhao, Li-Kun Chen, Jin-Yi Zhong*, and **Shi-Lu Chen***, Theoretical study of VX hydrolysis mechanism catalyzed by Phosphotriesterase mutant H254R, ***ChemistrySelect,* 2020,** 5, 8986–8991.
8	Ming-Jia Yu and **Shi-Lu Chen***, From Alkane to Alkene: The Inert Aliphatic C−H Bond Activation Presented by Binuclear Iron Stearoyl-CoA Desaturase with a Long di-Fe Distance of 6 Å, ***ACS Catalysis,* 2019,** 9, 4345-4359.
9	Shuo-Qi Sun and **Shi-Lu Chen***, How does Mo-dependent perchlorate reductase work in the decomposition of oxyanions?, ***Dalton Transactions,* 2019,** 48, 5683-5691.
10	Per E. M. Siegbahn*, **Shi-Lu Chen**, and Rong-Zhen Liao, Theoretical Studies of Nickel-Dependent Enzymes (***Review***), ***Inorganics 2019***, 7, 95.
11	Jian Yu, Hui-Xiang Sheng, Shuo-Wen Wang, Zhen-Hua Xu, Shi Tang* and **Shi-Lu Chen***, Copper-catalyzed radical cascades of *para*-quinone methides with AIBN and H_2O *via* α-cyanoalkylation by C–C bond cleavage: new access to benzofuran-2(3*H*)-ones, ***Chemical Communications,* 2019,** 55, 4578-4581.
12	Zhan Yan, Nai-Xing Wang*, Xue-Wang Gao, Jian-Li Li*, Yue-Hua Wu, Tong Zhang, **Shi-Lu Chen***, and Yalan Xing*, A Copper (II) Acetate Mediated Oxidative-Coupling of Styrenes and Ethers Through an Unactivated C(sp^3)-H BondFunctionalization, ***Advanced Synthesis & Catalysis,* 2019,** 361, 1007–1011.
13	Hang Wang, Pietro Rassu, Xiao Wang, Haiwei Li, Xiaorui Wang, Xiaoqi Wang, Xiao Feng, Anxiang Yin, Pengfei Li, Xu Jin, **Shi-Lu Chen***, Xiaojie Ma*, and Bo Wang*, An Iron metal-organic framework as highly efficient catalyst for ozone decomposition, ***Angew. Chem. Int. Ed.,* 2018,** 57, 16416-16420.
14	Jian-Nan Ji and **Shi-Lu Chen***, Asymmetric abstraction of two chemically-equivalent methylene hydrogens: significant enantioselectivity of endoperoxide presented by fumitremorgin B endoperoxidase, ***Phys. Chem. Chem. Phys.,* 2018,** 20, 26500-26505.
15	Ying Wang and **Shi-Lu Chen***, How is DMSP decomposed when catalyzed by RlDddP binuclear iron DMSP lyase?, ***Journal of Catalysis,* 2018,** 360, 1–8.
16	Xue-Wei Zhang, and **Shi-Lu Chen***, How does binuclear zinc amidohydrolase FwdA work in the initial step of methanogenesis: From formate to formyl-methanofuran, ***Journal of Inorganic Biochemistry***, **2018**, 185, 71 – 79.
17	Zeng-Zeng Li, Jian Yu, Liang-Neng Wang, **Shi-Lu Chen***, Rui-Long Sheng, Shi Tang*, Cascade radical cyclization/cross-coupling of halobenzamides by synergistic Cu/Fe catalysis: An access to 7-tert-alkylated isoquinolinediones, ***Tetrahedron***, **2018**, 74, 6558-6568.
18	Ming-jia Yu and **Shi-Lu Chen***, From NAD^+ to Ni Pincer Complex: A Significant Cofactor Evolution Presented by Lactate Racemase, ***Chemistry - A European Journal***, **2017**, 23, 7545 – 7557.
19	Jing-Xuan Su and **Shi-Lu Chen***, Significant electron transfer in heme catalysis: The case of chlorite dismutase, ***Journal of Catalysis,* 2017,** 348, 40–46.

20	Cui-Lan Lan and **Shi-Lu Chen***, The Decarboxylation of α,β-Unsaturated Acid Catalyzed by Prenylated FMN-Dependent Ferulic Acid Decarboxylase and the Enzyme Inhibition, ***The Journal of Organic Chemistry,*** **2016,** 81(19), 9289–9295.
21	Jian-Nan Ji and **Shi-Lu Chen***, μ_3-Oxo stabilized by three metal cations is a sufficient nucleophile for enzymatic hydrolysis of phosphate monoesters, ***Dalton Trans.,*** **2016,** 45, 2517–2522.
22	Qun Liu, Ze-Sheng Li, and **Shi-Lu Chen***, Metal-Embedded Graphene as Potential Counter Electrode for Dye-Sensitized Solar Cell, ***Ind. Eng. Chem. Res.***, **2016**, 55 (2), 455–462.
23	Xing-Wang Lan, Nai-Xing Wang*, Cui-Bing Bai, Cui-Lan Lan, Tong Zhang, **Shi-Lu Chen***, and Yalan Xing, Unactivated C(sp^3)-H Bond Functionalization of Alkyl Nitriles with Vinylarenes and Mechanistic Studies, ***Org. Lett.***, **2016**, 18, 5986−5989.
24	Shi Tang*, You-Lin Deng, Jie Li, Wen-Xin Wang, Ying-Chun Wang, Zeng-Zeng Li, Li Yuan, **Shi-Lu Chen***, and Rui-Long Sheng, Aerobic oxidative cyclization of benzamides *via meta*-selective C–H *tert*-alkylation: rapid entry to 7-alkylated isoquinolinediones, ***Chem. Commun.***, **2016**, 52, 4470-4473.
25	Rong-Zhen Liao*, **Shi-Lu Chen**, Per E. M. Siegbahn, Unraveling the Mechanism and Regioselectivity of the B_{12}-Dependent Reductive Dehalogenase PceA, ***Chemistry - A European Journal***, **2016**, *22(35)*, 12391–12399.
26	Hai-Mei Zhang and **Shi-Lu Chen***, Include Dispersion in Quantum Chemical Modeling of Enzymatic Reactions: The Case of Isoaspartyl Dipeptidase, ***J. Chem. Theory Comput.***, **2015**, 11(6), 2525-2535.
27	Bo Zou, Liang Hao, Lin-Yuan Fan, Zhi-Ming Gao, **Shi-Lu Chen***, Hui Li*, Chang-Wen Hu*, Highly efficient conversion of CO_2 at atmospheric pressure to cyclic carbonates with in *situ*-generated homogeneous catalysts from a copper-containing coordination polymer, ***Journal of Catalysis***, **2015**, 329, 119-129.
28	**Shi-Lu Chen***, Chemical Empiricism 2.0 at Age of Big Data: Large-scale Prediction of Reaction Pathways Based on Bond Dissociation Energies, ***Chinese J. Chem. Phys.***, ***2015***, 28(6), 674–680.
29	Nan Guo, Jin-Yi Zhong*, **Shi-Lu Chen***, Jing-Quan Liu, Qi Min, Rui-Xue Shi, Experimental and theoretical studies of hydrolysis of nerve agent sarin by binuclear zinc biomimetic catalysts, ***Chemical Physics***, **2015**, 457, 70-77.
30	Li-Na Yang, **Shi-Lu Chen***, Ze-Sheng Li*, How does the silicon element perform in JD-dyes: a theoretical investigation, ***J. Mater. Chem. A***, **2015**, 3, 8308–8315.
31	Xiaopeng Wang, Lixia Wang, Fei Zhao, Chuangang Hu, Yang Zhao, Zhipan Zhang*, **Shilu Chen***, Gaoquan Shi and Liangti Qu*, Monoatomic-thick graphitic carbon nitride dots on graphene sheets as an efficient catalyst in the oxygen reduction reaction, ***Nanoscale***, **2015**, 7, 3035–3042.
32	Li-Na Yang, Hong-Yan Zhou, Ping-Ping Sun, **Shi-Lu Chen***, Ze-Sheng Li*, A Promising Candidate with D-A-A-A Architecture as an Efficient Sensitizer for Dye-Sensitized Solar Cells, ***ChemPhysChem***, **2015**, 16, 601–606.
33	Rong-Zhen Liao*, **Shi-Lu Chen**, Per E. M. Siegbahn, Which Oxidation State Initiates Dehalogenation in the B_{12}-Dependent Enzyme NpRdhA: Co^{II}, Co^{I}, or Co^{0}, ***ACS***

	Catalysis, **2015**, 5, 7350–7358.
34	Xiaoyu Ma, Bo Zou, Minhua Cao*, **Shi-Lu Chen***, Changwen Hu*, Nitrogen-doped porous carbon monolith as a highly efficient catalyst for CO_2 conversion, ***J. Mater. Chem. A***, **2014**, 2, 18360–18366.
35	**Shi-Lu Chen***, Margareta R. A. Blomberg, Per E. M. Siegbahn*, An Investigation of Possible Competing Mechanisms for Ni-containing Methyl-Coenzyme M Reductase, ***Phys. Chem. Chem. Phys.***, **2014**, 16, 14029-14035.
36	Li-Na Yang, Zhu-Zhu Sun, Quan-Song Li, **Shi-Lu Chen***, Ze-Sheng Li*, Thomas A. Niehaus, Unsymmetrical Squaraine Dye Containing Dithieno[3,2-*b*:2′,3′-*d*]pyrrole as a π-spacer: a Potential Photosensitizer for Dye-Sensitized Solar Cells, ***Journal of Power Sources***, **2014**, 268, 137-145.
37	**Shi-Lu Chen***, Rong-Zhen Liao*, Phosphate Monoester Hydrolysis by Trinuclear Alkaline Phosphatase; DFT Study of Transition States and Reaction Mechanism, ***ChemPhysChem***, **2014**, 15, 2321–2330.
38	Ying-Nan Chi, Pan-Pan Shen, Feng-Yun Cui, Zheng-Guo Lin, **Shi-Lu Chen***, Chang-Wen Hu*, Symmetry Breaking of α-$[H_2W_{12}O_{40}]^{6-}$ Depends on the Transformation of Isopolyoxotungstates, ***Inorg. Chem.***, **2014**, 53, 5029–5036.
39	Shuo Sun, Ze-Sheng Li, **Shi-Lu Chen***, A dominant homolytic O–Cl bond cleavage with low-spin triplet-state Fe(IV)=O formed is revealed in the mechanism of heme-dependent chlorite dismutase, ***Dalton Transactions***, **2014**, 43, 973-981.
40	Li-Na Yang, Zhu-Zhu Sun, **Shi-Lu Chen***, Ze-Sheng Li*, Iodinated AlIII-Based Phthalocyanines are Promising Sensitizers for Dye-Sensitized Solar Cells; A Theoretical Comparison Between ZnII, MgII, and AlIII-Based Phthalocyanine Sensitizers, ***ChemPhysChem***, **2014**, *15*, 458-466.
41	**Shi-Lu Chen**, Li-Na Yang, Ze-Sheng Li*, How to design more efficient organic dyes for dye-sensitized solar cells? Adding more sp^2-hybridized nitrogen in the triphenylamine donor, ***Journal of Power Sources***, **2013**, *223*, 86-93.
42	Li-Na Yang, Zhu-Zhu Sun, **Shi-Lu Chen***, Ze-Sheng Li*, The effects of various anchoring groups on optical and electronic properties of dyes in dye-sensitized solar cells, ***Dyes and Pigments***, **2013**, *99*, 29-35.
43	**Shi-Lu Chen***, M. R. A. Blomberg, P. E. M. Siegbahn*, How Is Methane Formed and Oxidized Reversibly When Catalyzed by Ni-Containing Methyl-Coenzyme M Reductase?, ***Chemistry - A European Journal***, **2012**, *18(20)*, 6309-6315.
44	Fawang Chen, Xiaofang Li, Bo Wang, Tiegang Xu, **Shi-Lu Chen***, Peng Liu*, Changwen Hu*, Mechanism of the cycloaddition of carbon dioxide and epoxides catalyzed by Co-substituted 12-tungstenphosphate, ***Chemistry - A European Journal***, **2012**, *18(32)*, 9870-9876.
45	**Shi-Lu Chen***, Ze-Sheng Li, Wei-Hai Fang*, Theoretical investigation of astacin proteolysis, ***Journal of Inorganic Biochemistry***, **2012**, *111*, 70-79.
46	**Shi-Lu Chen***, M. R. A. Blomberg, P. E. M. Siegbahn*, How Is a Co-Methyl Intermediate Formed in the Reaction of Cobalamin-Dependent Methionine Synthase? Theoretical Evidence for a Two-Step Methyl Cation Transfer Mechanism, ***J. Phys. Chem. B***, **2011**, *115(14)*, 4066-4077.

47	Yue-Jie Ai, Rong-Zhen Liao, **Shi-Lu Chen**, Wei-Jie Hua, Wei-Hai Fang*, and Yi Luo*, Repair of DNA Dewar Photoproduct to (6-4) Photoproduct in (6-4) Photolyase, ***J. Phys. Chem. B***, **2011**, *115(37)*, 10976-10982.
48	P. E. M. Siegbahn*, M. R. A. Blomberg, **Shi-Lu Chen**, Significant van der Waals Effects in Transition Metal Complexes, ***J. Chem. Theory Comput.***, **2010**, *6(7)*, 2040-2044.
49	**Shi-Lu Chen***, V. Pelmenschikov, M. R. A. Blomberg, P. E. M. Siegbahn*, Is There a Ni-Methyl Intermediate in the Mechanism of Methyl-Coenzyme M Reductase, ***J. Am. Chem. Soc.***, **2009**, *131(29)*, 9912-9913.
50	**Shi-Lu Chen**, Wei-Hai Fang*, Fahmi Himo*, Reaction Mechanism of the Binuclear Zinc Enzyme Glyoxalase II – A Theoretical Study, ***Journal of Inorganic Biochemistry***, **2009**, *103*, 274-281.
51	**Shilu Chen**, Wei-Hai Fang*, Insights into photodissociation dynamics of acetaldehyde from ab initio calculations and molecular dynamics simulations, ***J. Chem. Phys.***, **2009**, *131(5),* 054306.
52	**Shi-Lu Chen**, Tiziana Marino, Wei-Hai Fang, Nino Russo*, Fahmi Himo*, Peptide Hydrolysis by the Binuclear Zinc Enzyme Aminopeptidase from Aeromonas proteolytica: A Density Functional Theory Study, ***J. Phys. Chem. B***, **2008**, *112(8)*, 2494-2500.
53	**Shi-Lu Chen**, Wei-Hai Fang, Fahmi Himo*, Technical Aspects of Quantum Chemical Modeling of Enzymatic Reactions: the Case of Phosphotriesterase, ***Theoretical Chemistry Accounts,*** **2008**, *120*, 515-522.
54	Jungwook Kim, Ping-Chuan Tsai, **Shi-Lu Chen**, Fahmi Himo*, Steven C. Almo*, Frank M. Raushel*, Structure of Diethyl Phosphate Bound to the Binuclear Metal Center of Phosphotriesterase, ***Biochemistry***, **2008**, *47(36),* 9497-9504.
55	**Shi-Lu Chen**, Wei-Hai Fang, Fahmi Himo*, Theoretical Study of the Phosphotriesterase Reaction Mechanism, ***J. Phys. Chem. B***, **2007**, *111(6)*, 1253-1255.
56	**Shi-Lu Chen**, Wei-Hai Fang*, Insights into Mechanistic Photodissociation of Acetyl Chloride by ab Initio Calculations and Molecular Dynamics Simulations, ***J. Phys. Chem. A***, **2007**, *111(38)*, 9355-9361.
57	**Shi-Lv Chen**, Wei-Hai Fang*, Insights into Photodissociation Dynamics of Propionyl Chloride from ab Initio Calculations and Molecular Dynamics Simulations, ***J. Phys. Chem. A***, **2006**, *110(3)*, 944-950.
58	**Shi-Lv Chen**, Fen Ding, Yu Liu, Hui-Chun Zhao*, Electrochemiluminescence of Terbium (III)-Two Fluoroquinolones- Sodium Sulfite System in Aqueous Solution, ***Spectrochimica Acta Part A***, **2006**, *64*, 130-135.
59	**Shi-Lv Chen**, Yu Liu, Hui-Chun Zhao*, Lin-Pei Jin, Zhong-Lun Zhang, Yan-Zhen Zheng, Determination of Norfloxacin Using a Terbium-Sensitized Electrogenerated Chemiluminescence Method, ***Luminescence***, **2006**, *21*, 20-25.
60	**Shilv Chen**, Huichun Zhao*, Xiaoli Wang, Xia Li, Linpei Jin, Determination of Trivalent Europium Using Flow Injection Chemiluminescence Method, ***Analytica Chimica Acta***, **2004**, *506*, 25-29.

61	**Shilv Chen**, Hongwu Ma, Huichun Zhao*, Ruiqing Feng, Linpei Jin, Terbium Sensitized Fluorescence Method for the Determination of Pazufloxacin Mesilate and Its Application, ***Analytical Sciences***, **2004**, *20*, 1075-1078.
62	**Shi-Lu Chen**, Hui-Chun Zhao*, Chun-Yan Sun, Ning Lian, and Lin-Pei Jin, A Study on Terbium Sensitized Chemiluminescence of Pipemidic Acid and Its Application, ***Analytical Letters***, **2002**, *35(10)*, 1705-1714.