

固体表面物理化学国家重点实验室 2004 年论文目录

A 类 国际刊物与书籍

综述文章:

- 1 Adsorption and reaction at electrochemical interfaces as probed by surface-enhanced Raman spectroscopy
Tian, ZQ; Ren, B
Annu Rev Phys Chem, 55(2004) 197 - 229

专著

- 1 《量子化学计算方法与应用》林梦海编著, 北京, 科学出版社
- 2 《结构化学》厦门大学化学系物构组编 林梦海等执笔, 北京, 科学出版社
- 3 《电化学》吴辉煌主编, 北京, 化学工业出版社

书籍章节

- 1 价键理论方法的研究进展与展望
吴玮, 宋凌春, 张乾二
《新世纪的物理化学—学科前沿与展望》(第二篇: 理论与计算化学) 梁文平, 杨俊林, 陈拥军, 李灿主编(国家自然科学基金委员会化学科学部组编), 科学出版社, 2004, p108-112
- 2 催化学科前沿与发展趋势浅议
王野, 袁友珠, 翁维正, 万惠霖
《新世纪的物理化学—学科前沿与展望》(第三篇: 催化科学) 梁文平, 杨俊林, 陈拥军, 李灿主编(国家自然科学基金委员会化学科学部组编), 科学出版社, 2004, p133-141
- 3 腐蚀电化学及研究方法的前沿和趋势
林昌健
《新世纪的物理化学—学科前沿和展望》(第六篇: 电科学) 梁文平, 杨俊林, 陈拥军, 李灿主编(国家自然科学基金委员会化学科学部组编), 科学出版社, 2004, p 311-315
- 4 纳米材料原子排列结构层次的电化学催化
孙世刚
《新世纪的物理化学—学科前沿与展望》(第六篇: 电化学) 梁文平, 杨俊林, 陈拥军, 李灿主编(国家自然科学基金委员会化学科学部组编), 科学出版社, 2004, p321-324
- 5 初探纳米电化学之发展
田中群, 毛秉伟, 向娟, 吴德印
《新世纪的物理化学—学科前沿与展望》(第六篇: 电化学) 梁文平, 杨俊林, 陈拥军, 李灿主编(国家自然科学基金委员会化学科学部组编), 科学出版社, 2004, p333-341

- 6 微米尺度固液体系的物理化学问题和创新契机
田昭武, 林华水, 周勇亮, 田中群, 蒋利民
《新世纪的物理化学—学科前沿与展望》(第十篇: 物理化学中的方法与技术) 梁文平,
杨俊林, 陈拥军, 李灿主编(国家自然科学基金委员会化学科学部组编), 科学出版社,
2004, p496-501

论文:

- 1 Bis[tetrakis(triphenylphosphine-kappa P)-silver(I)] di-mu-trifluoroacetato-kappa O-4 : O
'-bis[bis(trifluoroacetato-kappa O)-stannate(IV)]
Yang, SY; Xie, ZX; Ng, SW
Acta Crystallogr C, 60(2004) M123 - M125 Part 3
- 2 A simple and effective route for the synthesis of crystalline silver nanorods and nanowires
Hu, JQ; Chen, Q; Xie, ZX; Han, GB; Wang, RH; Ren, B; Zhang, Y; Yang, ZL; Tian, ZQ
Adv Funct Mater, 14 (2) (2004) 183 - 189
- 3 Synthesis of single-crystalline ZnO polyhedral submicrometer-sized hollow beads using
laser-assisted growth with ethanol droplets as soft templates
Jiang, ZY; Xie, ZX; Zhang, XH; Lin, SC; Xu, T; Xie, SY; Huang, RB; Zheng, LS
Adv Mater, 16 (11) (2004) 904 - 907
- 4 Laser-induced formation of metal-peroxide linkages on the surface of lanthanum
sesquioxide under oxygen
Weng, WZ; Wan, HL; Li, JM; Cao, ZX
Angew. Chem. Int. Ed. , 43 (8) (2004) 975 - 977
- 5 The magnitude of hyperconjugation in ethane: A perspective from ab initio valence bond
theory
Mo, YR; Wu, W; Song, LC; Lin, MH; Zhang, Q; Gao, JL
Angew. Chem. Int. Ed. , 43 (15) (2004) 1986 - 1990
- 6 A three-dimensional coordination polymer: poly-[mu(7)-1,2,4,5-
benzenetetracarboxylato-bis(N,N-dimethylformamide)dizinc(II)]
Yang, SY; Long, LS; Huang, RB; Zheng, LS; Ng, SW
Appl Organomet Chem , 18 (2) (2004) 91 - 92
- 7 [Diaqua bis(2,2 '-bipyridine)(mu-naphthalene-1,4,5,8-tetracarboxylato)]dizinc(II)
tetrahydrate
Zhao, XJ; Tao, J
Appl Organomet Chem , 18 (9) (2004) 491 - 492
- 8 The hydroxyl species and acid sites on diatomite surface: a combined IR and Raman study
Yuan, P; Wu, DQ; He, HP; Lin, ZY
Appl Surf Sci , 227 (38356) (2004) 30 - 39

- 9 Liquid crystalline behaviour of chitooligosaccharides
Dong, YM; Wang, HW; Zheng, WY; Zhao, YQ; Bi, DX; Zhao, LJ; Li, XF
Carbohydr Polym , 57 (3) (2004) 235 - 240
- 10 The graphite arc-discharge in the presence of CCl₄: Chlorinated carbon clusters in relation with fullerenes formation
Gao, F; Xie, SY; Ma, ZJ; Feng, YQ; Huang, RB; Zheng, LS
Carbon, 42 (10) (2004) 1959 - 1963
- 11 Low temperature solvothermal synthesis of crumpled carbon nanosheets
Kuang, Q; Xie, SY; Jiang, ZY; Zhang, XH; Xie, ZX; Huang, RB; Zheng, LS
Carbon, 42 (38573) (2004) 1737 - 1741
- 12 Effect of zirconia phase on the reduction behaviour of highly dispersed zirconia-supported copper oxide
Zhao, YB; Tao, KY; Wan, HL
Catal. Comm., 5 (5) (2004) 249 - 252
- 13 Micelle effect of disulfonated cetyldiphenyl phosphine in biphasic hydroformylation of higher olefins
Peng, QR; Liao, XL; Yuan, YZ
Catal. Comm., 5 (8) (2004) 447 - 451
- 14 Iron-based heterogeneous catalysts for epoxidation of alkenes using molecular oxygen
Liang, J; Zhang, QH; Wu, HL; Meng, GY; Tang, QH; Wang, Y
Catal. Comm., 5 (11) (2004) 665 -669
- 15 Direct oxidation of propane to acrolein over MCM41-supported MoVTe mixed oxide catalysts
Chen, LQ; Liang, J; Weng, WZ; Wang, Y; Wan, HL; Vedrine, JC
Catal. Comm., 5 (11) (2004) 697 -701
- 16 Selective hydrogenation of trans-cinnamaldehyde over SiO₂-supported Co-Ir bimetallic catalysts
Zhu, MX; Wang, XQ; Lai, JY; Yuan, YZ
Catal Lett, 98 (4) (2004) 247 - 254
- 17 SBA-15-supported iron phosphate catalyst for partial oxidation of methane to formaldehyde
Wang, Y; Wang, XX; Su, Z; Guo, Q; Tang, QH; Zhang, QH; Wan, HL
Catal Today , 93-95(2004) 155 - 161
- 18 Characterizations of cobalt oxide nanoparticles within faujasite zeolites and the formation of metallic cobalt
Tang, QH; Zhang, QH; Wang, P; Wang, Y; Wan, HL
Chem Mater, 16 (10) (2004) 1967 - 1976

- 19 CO₂-Exchanged faujasite zeolites as efficient heterogeneous catalysts for epoxidation of styrene with molecular oxygen
Tang, QH; Wang, Y; Liang, J; Wang, P; Zhang, QH; Wan, HL
Chem. Comm., (4)(2004)440-441

- 20 Synthesis of silver nanotubes by electroless deposition in porous anodic aluminium oxide templates
Zhang, SH; Xie, ZX; Jiang, ZY; Xu, X; Xiang, J; Huang, RB; Zheng, LS
Chem. Comm., (9) (2004) 1106 - 1107

- 21 Iron-catalysed propylene epoxidation by nitrous oxide: dramatic shift of allylic oxidation to epoxidation by the modification with alkali metal salts
Wang, XX; Zhang, QH; Guo, Q; Lou, YC; Yang, LJ; Wang, Y
Chem. Comm., (13) (2004) 1396 - 1397

- 22 Novel synthesis of FAU-type zeolite membrane with high performance
Cheng, ZL; Gao, EQ; Wan, HL
Chem. Comm., (15) (2004) 1718 - 1719

- 23 Glow discharge growth of SnO₂ nano-needles from SnH₄
Wang, CF; Xie, SY; Lin, SC; Cheng, X; Zhang, XH; Huang, RB; Zheng, LS
Chem. Comm., (15) (2004) 1766 - 1767

- 24 Simple metal oxides as efficient heterogeneous catalysts for epoxidation of alkenes by molecular oxygen
Liang, J; Tang, QH; Meng, GY; Wu, HL; Zhang, QH; Wang, Y
Chem. Lett., 33 (9) (2004) 1140 - 1141

- 25 Selective intermolecular zero-quantum coherence in high-resolution NMR under inhomogeneous fields
Chen, Z; Hou, T; Chen, ZW; Hwang, DW; Hwang, LP
Chem. Phys. Lett., 386 (38355) (2004) 200 - 205

- 26 Ordered silver adlayer formation by surface-induced dissociation of a coordination complex precursor on Au(111) and Au(100) surfaces
Xu, XM; Zhong, HP; Zhang, HM; Mo, YR; Xie, ZX; Long, LS; Zheng, LS; Mao, BW
Chem. Phys. Lett., 386 (38448)(2004)254-258

- 27 Theoretical study of dissociative potential energy curves and photodissociation mechanisms of the Mg⁺-pyridine complex in the low-lying states
Guo, C; Cao, ZX; Zhang, QN
Chem. Phys. Lett., 386 (38448) (2004) 448-453

- 28 Adsorbate lone-pair-electron stimulated charge transfer between surface dangling bonds: methanol chemisorption on Si(111)-7 x 7
Xu, X; Wang, CJ; Xie, ZX; Lu, X; Chen, MS; Tanaka, K

- Chem. Phys. Lett., 388 (38355) (2004) 190 -194
- 29 Beyond the intradimer [2+2] cycloaddition chemistry of ethylene on Si(100): theoretical evidence on the occurrence of interdimer reaction
Lu, X; Zhu, MP
Chem. Phys. Lett., 393 (38355) (2004) 124 - 127
- 30 The formation of an enynic-like intermediate in diacetylene binding on Si(100)-2 x 1
Huang, HG; Lu, X; Xiang, CL; Teo, TL; Lai, YH; Xu, GQ
Chem. Phys. Lett., 398 (38355) (2004) 11 - 14
- 31 Self-assembly of normal alkanes on the Au(111) surfaces
Zhang, HM; Xie, ZX; Mao, BW; Xu, X
Chem-Eur J , 10 (6) (2004) 1415 - 1422
- 32 Effects of chain length and Au spin-orbit coupling on $3(\pi \pi^*)$ emission from bridging C-n(2-) units: Theoretical characterization of spin-forbidden radiative transitions in metal-capped one-dimensional carbon chains [H₃PAu(C≡C)(n)AuPH₃]
Cao, ZX; Zhang, Q
Chem-Eur J , 10 (8) (2004) 1920 - 1925
- 33 The ground and excited states of polyenyl radicals C_{2n}H_{2n+1} (n=2-13): A valence bond study
Luo, Y; Song, LC; Wu, W; Danovich, D; Shaik, S
Chemphyschem, 5 (4) (2004) 515 - 528
- 34 Peroxomolybdate(VI)-citrate and -malate complex interconversions by pH-dependence. Synthetic, structural and spectroscopic studies
Zhou, ZH; Hou, SY; Wan, HL
Dalton T, (9) (2004) 1393 - 1399
- 35 Structural, electrochemical and thermal properties of LiNi_{0.8-y}Ti_yCo_{0.2}O₂ as cathode materials for lithium ion battery
Liu, HS; Li, J; Zhang, ZR; Gong, ZL; Yang, Y
Electrochim. Acta., 49 (7) (2004) 1151 - 1159
- 36 In situ FTIRS and EQCM studies of glycine adsorption and oxidation on Au(111) electrode in alkaline solutions
Zhen, CH; Sun, SG; Fan, CJ; Chen, SP; Mao, BW; Fan, YJ
Electrochim. Acta., 49(8) (2004) 1249 - 1255
- 37 Kinetics of dissociative adsorption of ethylene glycol on Pt(100) electrode surface in sulfuric acid solutions
Fan, YJ; Zhou, ZY; Zhen, CH; Fan, CH; Sun, SG
Electrochim. Acta., 49 (26) (2004) 4659 - 4666

- 38 Electrodeposition of Sb on Au(100) at underpotentials: structural transition involving expansion of the substrate surface
Yan, JW; Wu, Q; Shang, WH; Mao, BW
Electrochem Commun , 6 (8) (2004) 843 – 848
- 39 Origin of deterioration for LiNiO₂ cathode material during storage in air
Liu, HS; Zhang, ZR; Gong, ZL; Yang, Y
Electrochem Solid St , 7 (7) (2004) A190 - A193
- 40 Hydrothermal syntheses, crystal structures and photoluminescent properties of three metal-cluster based coordination polymers containing mixed organic ligands
Tao, J; Yin, X; Wei, ZB; Huang, RB; Zheng, LS
Eur. J. Inorg. Chem., (1) (2004)125-133
- 41 Ammonium barium citrato peroxotitanate(IV) Ba₂(NH₄)₂[Ti₄(O₂)₄(Hcit)₂(cit)₂] \cdot 10H₂O: a molecular precursor of stoichiometric BaTi₂O₅
Deng, YF; Zhou, ZH; Wan, HL; Tsai, KR
Inorg. Chem. Comm., 7 (2) (2004) 169 - 172
- 42 Synthesis of alpha-tellurium dioxide nanorods from elemental tellurium by laser ablation
Jiang, ZY; Xie, ZX; Zhang, XH; Xie, SY; Huang, RB; Zheng, LS
Inorg. Chem. Comm., 7 (2) (2004) 179 - 181
- 43 Enzymatic mechanism of Fe-only hydrogenase: Density functional study on H-H making/breaking at the diiron cluster with concerted proton and electron transfers
Zhou, TJ; Mo, YR; Liu, AM; Zhou, ZH; Tsai, KR
Inorg. Chem., 43 (3) (2004) 923 - 930
- 44 A well-resolved uudd cyclic water tetramer in the crystal host of [Cu(adipate)(4,4-bipyridine)] \cdot (H₂O)₂
Long, LS; Wu, YR; Huang, RB; Zheng, LS
Inorg. Chem., 43 (13) (2004)3798-3800
- 45 Synthesis and characterization of a tetrazolate-bridged coordination framework encapsulating D_{2h}-symmetric cyclic (H₂O)₄ cluster arrays
Tao, J; Ma, ZJ; Huang, RB; Zheng, LS
Inorg. Chem., 43 (20) (2004)6133-6135
- 46 pH-dependent isolations and spectroscopic, structural, and thermal studies of titanium citrate complexes
Deng, YF; Zhou, ZH; Wan, HL
Inorg. Chem., 43(20)(2004)6266-6273
- 47 A density functional study of the structures and energies of C_nP₅⁻ (n=1-7) clusters
Chen, MD; Liang, H; Liu, MH; Zhang, QE; Au, CT
Int J Mass Spectrom , 232 (2) (2004) 165 - 170

- 48 Applications of graphic method to C-20, C-60, and achiral single-wall nanotubes
Zhang, LL; Wu, W; Mo, YR; Mang, Q
Int. J Quantum Chem., 98 (1) (2004) 51 - 58
- 49 Linear and nonlinear feature of electronic excitation energy in carbon chains HC_{2n+H-1} and HC_{2nH}
Zhang, CJ; Cao, ZX; Wu, HS; Zhang, QR
Int. J Quantum Chem., 98 (3) (2004) 299 - 308
- 50 Studies on glass transition temperature of chitosan with four techniques
Dong, YM; Ruan, YH; Wang, HW; Zhao, YG; Bi, DX
J Appl Polym Sci , 93 (4) (2004) 1553 – 1558
- 51 High-resolution NMR spectra in inhomogeneous fields via IDEAL (intermolecular dipolar-interaction enhanced all lines) method
Chen, Z; Chen, ZW; Zhong, JH
J. Am. Chem. Soc., 126 (2) (2004) 446 - 447
- 52 Charge transfer in the electron donor-acceptor complex BH_3NH_3
Mo, YR; Song, LC; Wu, W; Zhang, QN
J. Am. Chem. Soc., 126 (15) (2004) 3974 - 3982
- 53 Synthesis and properties of tadpole-shaped gold nanoparticles
Hu, JQ; Zhang, Y; Liu, B; Liu, JX; Zhou, HH; Xu, YF; Jiang, YX; Yang, ZL; Tian, ZQ
J. Am. Chem. Soc., 126 (31) (2004) 9470 - 9471
- 54 Valence bond calculations of hydrogen transfer reactions: A general predictive pattern derived from theory
Su, PF; Song, LC; Wu, W; Hiberty, PC; Shark, S
J. Am. Chem. Soc., 126 (41) (2004) 13539 - 13549
- 55 Properties of fullerene[50] and D-5h decachlorofullerene[50]: A computational study
Lu, X; Chen, ZF; Thiel, W; Schleyer, PV; Huang, RB; Zheng, LS
J. Am. Chem. Soc., 126 (45) (2004) 14871 - 14878
- 56 Behavior of active sites on Cr-MCM-41 catalysts during the dehydrogenation of propane with CO_2
Takehira, K; Ohishi, Y; Shishido, T; Kawabata, T; Takaki, K; Zhang, QH; Wang, Y
J Catal , 224 (2) (2004) 404 -416
- 57 Partial oxidation of methane to H₂ and CO over Rh/SiO₂ and Ru/SiO₂ catalysts
Yan, QG; Wu, TH; Weng, WZ; Toghiani, H; Toghiani, RK; Wan, HL; Pittman, CU
J Catal , 226 (2) (2004) 247 - 259

- 58 CuCl₂ immobilized on amino-functionalized MCM-41 and MCM-48 and their catalytic performance toward the vapor-phase oxy-carbonylation of methanol to dimethylcarbonate
Yuan, YZ; Cao, W; Weng, WZ
J Catal , 228 (2) (2004) 311 -320
- 59 Abnormal IR effects of Pt nanostructured surfaces upon CO chemisorption due to interaction and electron-hole damping
Wu, CX; Lin, H; Chen, YJ; Li, WH; Sun, SG
J Chem Phys, 121 (3) (2004) 1553 – 1556
- 60 The extended Perdew-Burke-Ernzerhof functional with improved accuracy for thermodynamic and electronic properties of molecular systems
Xu, X; Goddard, WA
J Chem Phys, 121 (9) (2004) 4068 - 4082
- 61 A density functional study on nitrogen-doped carbon clusters C_nN₃- (n=1-8)
Chen, MD; Liu, JW; Dang, L; Zhang, Q; Au, CT
J Chem Phys, 121 (23) (2004) 11661 – 11667
- 62 A practical valence bond method: A configuration interaction method approach with perturbation theoretic facility
Song, LC; Wu, W; Zhang, Q; Shaik, S
J Comput Chem, 25 (4) (2004) 472 - 478
- 63 Enhanced IR absorption of CO adsorbed on Pd nanoparticles embedded in the mesoporous molecular sieve SBA-15
Jiang, YX; Ding, N; Sun, SG
J Electroanal Chem, 563 (1) (2004) 15 - 21
- 64 In situ rapid-scan time-resolved microscope FTIR spectroelectrochemistry: study of the dynamic processes of methanol oxidation on a nanostructured Pt electrode
Zhou, ZY; Tian, N; Chen, YJ; Chen, SP; Sun, SG
J Electroanal Chem, 573 (1) (2004) 111 - 119
- 65 An investigation of the adsorption of pyrazine and pyridine on nickel electrodes by in situ surface-enhanced Raman spectroscopy
Huang, QJ; Lin, XF; Yang, ZL; Hu, JW; Tian, ZQ
J Electroanal Chem, 563 (1) (2004) 121 – 131
- 66 Catalyst microstructure examination of PEMFC membrane electrode assemblies vs. time
Cheng, X; Chen, L; Peng, C; Chen, ZW; Zhang, Y; Fan, QB
J Electrochem Soc, 151 (1) (2004) A48 - A52
- 67 Comparison of electrochemical and surface properties of bare and TiO₂-coated LiNi_{0.8}Co_{0.2}O₂ electrodes
Zhang, ZR; Liu, HS; Gong, ZL; Yang, Y

- J Electrochem Soc, 151 (4) (2004) A599 - A603
- 68 Syntheses, crystal structures and biological relevance of glycolato and S-lactato molybdates
Zhou, ZH; Hou, SY; Cao, ZX; Wan, HL; Ng, SW
J Inorg Biochem , 98 (6) (2004) 1037 - 1044
- 69 Speciation and transformation of Co(II)/Ni(II)-citrate-imidazole ternary system - synthesis, spectroscopic and structural studies
Deng, YF; Zhou, ZH; Cao, ZX; Tsai, KR
J Inorg Biochem , 98 (6) (2004) 1110 - 1116
- 70 Enantiomeric and mesomeric mandelate complexes of molybdenum - on their stereospecific formations and absolute configurations
Zhou, ZH; Zhao, H; Tsai, KR
J Inorg Biochem , 98 (11) (2004) 1787 - 1794
- 71 Separation and characterization of different signals from intermolecular three-spin orders in solution NMR
Chen, Z; Chen, ZW; Hwang, DW; Zhong, JH; Hwang, LP
J Magn Reson, 171 (2) (2004) 244 - 252
- 72 Fabrication of core-shell Au-Pt nanoparticle film and its potential application as catalysis and SERS substrate
Lu, LH; Sun, GY; Zhang, HJ; Wang, HS; Xi, SQ; Hu, JQ; Tian, ZQ; Chen, R
J Mater Chem , 14 (6) (2004) 1005 - 1009
- 73 Ab initio calculations of the formation energies of lithium intercalations in SnSb
Hou, ZF; Li, A; Zhu, ZZ; Huang, MC; Yang, Y
J Mater Sci Technol , 20 (6) (2004) 743 - 745
- 74 A new efficient chiral iridium catalyst for asymmetric transfer hydrogenation of ketones
Li, YY; Zhang, H; Chen, JS; Liao, XL; Dong, ZR; Gao, JX
J Mol Catal A-Chem, 218 (2) (2004) 153 - 156
- 75 Immobilization of rhodium complexes ligated with triphenylphosphine analogs on amino-functionalized MCM-41 and MCM-48 for 1-hexene hydroformylation
Peng, QR; Yang, Y; Yuan, YZ
J Mol Catal A-Chem, 219 (1) (2004) 175 - 181
- 76 A density functional theory study of germanium Ge-11 clusters
Luo, HB; Li, XB; Zhang, QE; Chen, MD; Cheng, YK
J. Mol. Struct. (Theochem), 674 (38355) (2004) 83 - 86
- 77 Spectroscopic studies of the conformational properties of naphthoyl chitosan in dilute solutions
Wu, YS; Seo, TH; Maeda, S; Dong, YM; Sasaki, T; Irie, S; Sakurai, K

- J Polym Sci Pol Phys, 42 (14) (2004) 2747 - 2758
- 78 Electrochemical performance and spectroscopic characterization of TiO₂-coated LiNi_{0.8}CO_{0.2}O₂ cathode materials
Zhang, ZR; Liu, HS; Gong, ZL; Yang, Y
J Power Sources, 129 (1) (2004) 101 - 106
- 79 Preparation and self-assembly of copper nanoparticles via discharge of copper rod electrodes in a surfactant solution: a combination of physical and chemical processes
Xie, SY; Ma, ZJ; Wang, CF; Lin, SC; Jiang, ZY; Huang, RB; Zheng, LS
J Solid State Chem, 177 (10) (2004) 3743 - 3747
- 80 Studies of solvation free energies of methylammoniums and irregular basicity ordering of methylamines in aqueous solution by a combined discrete-continuum model
Cao, ZJ; Lin, MH; Zhang, QN; Mo, YR
J. Phys. Chem. A., 108 (19) (2004) 4277 - 4282
- 81 Theoretical study of arsenic-doped carbon clusters C(n)A(s-) (n=1-11)
Liu, JW; Chen, MD; Zheng, LS; Zhang, QE; Au, CT
J. Phys. Chem. A., 108 (26) (2004) 5704 - 5709
- 82 VBPCM: A valence bond method that incorporates a polarizable continuum model
Song, LC; Wu, W; Zhang, QN; Shaik, S
J. Phys. Chem. A., 108 (28) (2004) 6017 - 6024
- 83 Assessment of Handy-Cohen optimized exchange density functional (OPTX)
Xu, X; Goddard, WA
J. Phys. Chem. A., 108 (40) (2004) 8495 - 8504
- 84 Time-dependent density functional theory investigation of electronic excited states of tetraoxaporphyrin dication and porphycene
Wan, J; Ren, YL; Wu, JM; Xu, X
J. Phys. Chem. A., 108 (43) (2004) 9453 - 9460
- 85 Electrochemical and surface-enhanced Raman spectroscopic studies on the adsorption and electrooxidation of C-1 molecules on a roughened Rh electrode
Lin, XF; Ren, B; Tian, ZQ
J. Phys. Chem. B., 108 (3) (2004) 981 - 986
- 86 Electrochemical growth of three-dimensional nanostripe architecture of antimony on Cu(100)
Wu, JH; Yan, JW; Xie, ZX; Xue, QK; Mao, BW
J. Phys. Chem. B., 108 (9) (2004) 2773 - 2776
- 87 Producing reactive species on Si(100), Ge(100), and Si(111) surfaces by attachments of diacetylenes

- Lu, X; Zhu, MP; Wang, XL; Zhang, QN
J. Phys. Chem. B., 108 (14) (2004) 4478 – 4484
- 88 Spherical double electric layer structure and unprecedented high stability of the P20O20 cage and its anionic endohedral complex Na-@P20O20
Wang, YJ; Xu, JQ; Cao, ZX; Zhang, QN
J. Phys. Chem. B., 108 (15) (2004) 4579 - 4581
- 89 Diradical mechanisms for the cycloaddition chemistry of ethylene on X(100) surfaces (X = C, Si, and Ge)
Lu, X; Zhu, MP; Wang, XL
J. Phys. Chem. B., 108 (22) (2004) 7359 - 7362
- 90 First spectroscopic observation of peroxocarbonate/peroxodicarbonate in molten carbonate
Chen, LJ; Lin, CJ; Zuo, J; Song, LC; Huang, CM
J. Phys. Chem. B., 108 (23) (2004) 7553 - 7556
- 91 In situ microscope FTIRS studies of CO adsorption on an individually addressable array of nanostructured Pt microelectrodes - an approach of combinatorial analysis of anomalous IR properties
Gong, H; Sun, SG; Chen, YJ; Chen, SP
J. Phys. Chem. B., 108 (31) (2004) 11575 - 11584
- 92 Surface-enhanced Raman scattering from bare Zn electrode
Gu, RA; Shen, XY; Liu, GK; Ren, B; Tian, ZQ
J. Phys. Chem. B., 108 (45) (2004) 17519 - 17522
- 93 Electrochemical performance and surface properties of bare and TiO₂-coated cathode materials in lithium-ion batteries
Zhang, ZR; Gong, ZL; Yang, Y
J. Phys. Chem. B., 108 (45) (2004) 17546 - 17552
- 94 Theoretical consideration on preparing silver particle films by adsorbing nanoparticles from bulk colloids to an air-water interface
Hu, JW; Han, GB; Ren, B; Sun, SG; Tian, ZQ
Langmuir, 20 (20) (2004) 8831 - 8838
- 95 Anomalous IR properties of nanostructured films created by square wave potential on an array of pt microelectrodes: An in situ microscope FTIRS study of CO adsorption
Chen, YJ; Sun, SG; Chen, SP; Li, JT; Gong, H
Langmuir, 20 (23) (2004) 9920 - 9925
- 96 Can the nitroso Ene reaction proceed concertedly?
Lu, X
Organic Letters, 6 (16) (2004) 2813 - 2815

- 97 Transformation of maleato manganese(II): temperature effect and coordination modes
Chen, HB; Zhang, H; Yang, JM; Zhou, ZH
Polyhedron, 23 (6) (2004) 987 - 991
- 98 The X3LYP extended density functional for accurate descriptions of nonbond interactions, spin states, and thermochemical properties
Xu, X; Goddard, WA
Proc. Nati. Acad. Sci. USA, 101 (9) (2004) 2673 - 2677
- 99 Capturing the labile fullerene[50] as C₅₀Cl₁₀
Xie, SY; Gao, F; Lu, X; Huang, RB; Wang, CR; Zhang, X; Liu, ML; Deng, SL; Zheng, LS
Science, 304 (5671) (2004) 699 - 699
- 100 Preparation and performance of nickel-tin alloys used as anodes for lithium-ion battery
Dong, QF; Wu, CZ; Jin, MG; Huang, ZC; Zheng, MS; You, JK; Lin, ZG
Solid State Ionics, 167 (38354) (2004) 49 - 54
- 101 A comparative study of LiNi_{0.8}Co_{0.2}O₂ cathode materials modified by lattice-doping and surface-coating
Liu, HS; Zhang, ZR; Gong, ZL; Yang, Y
Solid State Ionics, 166 (38415) (2004) 317 - 325
- 102 Characterization of diatomaceous silica by Raman spectroscopy
Yuan, P; He, HP; Wu, DQ; Wang, DQ; Chen, LJ
Spectrochim Acta A, 60 (12) (2004) 2941 - 2945
- 103 Theoretical differential Raman scattering cross-sections of totally-symmetric vibrational modes of free pyridine and pyridine-metal cluster complexes
Wu, DY; Hayashi, M; Lin, SH; Tian, ZQ
Spectrochim Acta A, 60 (38354) (2004) 137 - 146
- 104 Spectroscopic studies on the interactions between a bioactive diperoxovanadate complex and pyridine
Yu, XY; Cai, SH; Chen, Z
Spectrochim Acta A, 60 (38354) (2004) 391 - 396
- 105 Influence of calcination temperature on the primary products of methane partial oxidation to synthesis gas over Rh/Al₂O₃ catalyst
Weng, WZ; Luo, CR; Li, JM; Lin, HQ; Wan, HL
Stud Surf Sci Catal, 147(2004) 145 - 150
- 106 Superior catalytic activity of nano-sized metallic cobalt inside faujasite zeolite for Fischer-Tropsch synthesis
Tang, QH; Wang, Y; Wang, P; Zhang, QH; Wan, HL
Stud Surf Sci Catal, 147(2004) 325 - 330

- 107 Effect of support structure on methane combustion over PdO/ZrO₂
Yang, LF; Hu, YX; Jin, D; He, XE; Shi, CK; Cai, JX
Stud Surf Sci Catal, 147(2004) 469 - 474
- 108 The catalytic combustion of CH₄ over Pd-Zr/HZSM-5 catalyst with enhanced stability and activity
Shi, CK; Yang, LF; Cai, JX
Stud Surf Sci Catal, 147(2004) 475 - 480
- 109 Selective oxidation of CH₄ to CH₃OH using the Catalytica (bpym)PtCl₂ catalyst: a theoretical study
Xu, X; Fu, G; Goddard, WA; Periana, RA
Stud Surf Sci Catal, 147(2004) 499 - 504
- 110 Dehydro-aromatization of CH₄ over W-Mn(or Zn, Ga, Mo, Co)/HZSM-5(or MCM-22) catalysts
Huang, LQ; Yuan, YZ; Zhang, HB; Xiong, ZT; Zeng, JL; Lin, GD
Stud Surf Sci Catal, 147(2004) 565 - 570
- 111 Effect of support on performance of MoVTeO catalyst for selective oxidation of propane to acrolein
Huang, CJ; Guo, W; Yi, XD; Weng, WZ; Wan, HL
Stud Surf Sci Catal, 147(2004) 661 - 666
- 112 Infrared study of the reaction pathways for the selective oxidation of propane to acrolein over MOPO/SiO₂ catalyst
Yi, XD; Weng, WZ; Huang, CJ; He, YM; Guo, W; Wan, HL
Stud Surf Sci Catal, 147(2004) 667 - 672
- 113 Asymmetric transfer hydrogenation of aromatic ketones catalyzed by the iridium hydride complex under ambient conditions
Chen, JS; Li, YY; Dong, ZR; Li, BZ; Gao, JX
Tetrahedron Lett, 45 (45) (2004) 8415 - 8418
- 114 The correlation between metal oxidation state and bond valence parameters for M-O bonds (M = V, Fe and Cu). A simple method to search for the metal oxidation-state independent parameter pairs
Hu, SZ; Zhou, ZH
Z Kristallogr, 219 (10) (2004) 614 - 620
- 115 Partial oxidation of methane to syngas over Rh/SiO₂ catalyst using on-line MS
Wu, TH; Yan, QG; Mao, FL; Niu, ZJ; Zhang, QN; Li, ZL; Wan, HL
Catal Today, 93-95 (2004) 121 -127
- 116 Effects of preparation methods of LiNi_{0.8}Co_{0.2}O₂ cathode materials on their morphology and electrochemical performance

Gong, ZL; Liu, HS; Guo, XJ; Zhang, ZR; Yang, Y
J Power Sources, 136 (1) (2004) 139 - 144

117 Intermolecular double-quantum coherence MR microimaging of pig tail with unique image contrast

Hou, T; Chen, Z; Hwang, DW; Zhong, JH; Hwang, LP
Magn Reson Imaging, 22 (4) (2004) 543 - 550