## 学术论文(*通信作者)

**2012**

64. 吴婧,**巫翔**,朱峰,张倩,秦善(2012): 掺 Fe 和 V 的金红石电子结构的第一性原理计算研究，岩石矿物学报，在印.
63. 赖潇静,李奇,徐伟,陈栋梁,**巫翔**,秦善(2012): 金刚石中微量元素的同步辐射 X 射线荧光分析，地质科技情报，在印.
62. Wu Y, Zhang Q, **Wu X***, Qin S, and Liu J (2012): High pressure structural study of β-$Ti_3O_5$: X-ray diffraction and Raman spectroscopy, Journal of solid state chemistry, accepted.
61. Zhu F, **Wu X***, and Qin S (2012): First-principles investigation on high-pressure structural evolution of $MnTiO_3$, Solid State Communications, online (http://dx.doi.org/10.1016/j.ssc.2012.03.014).
60. Wu Y, **Wu X***, and Qin S (2012): Pressure-induced phase transition of $Fe_2TiO_4$: X-ray diffraction and Mössbauer spectroscopy, Journal of solid state chemistry, 185, 72-75.
59. Gu TT, **Wu X**, Qin S, Liu J, Li YC, and Zhang YF (2012): High-Pressure and High-Temperature in situ X-ray diffraction study of $FeP_2$ up to 70 GPa, Chinese Physical Letters, 29, 026102:1-3.
58. Zhang LJ, Wang JQ, Li J, Zhou J, Cai WP, Chen J, Xu W, **Wu X**, Jiang Z, Zhang S, and Wu ZY(2012): High-Tc ferromagnetism in a Co-doped ZnO system dominated by the formation of a zince-blende type Co-rich ZnCoO phase. Chemical Communication, 48, 91-93.

**2011 年**

57. **Wu X***, Mookherjee M, Gu T T, and Qin S (2011): Elasticity and anisotropy of iron-nickel phosphides at high pressures, Geophysical Research Letters, 38, L20301.
56. Gu T T, **Wu X***, Qin S, and Dubrovinsky L (2011): In situ high-pressure study of FeP: Implications for planetary cores, Physics of Earth and Planetary Interiors, 184, 154-159.
55. **Wu X***, Qin S, and Dubrovinsky L (2011): Investigation into high-pressure behaviour of $MnTiO_3$: X-ray diffraction and Raman spectroscopy with diamond anvil cells, Geoscience Frontiers, 2, 107-114.
54. **Wu X***, Qin S, Gu TT, Yang J, and Manthilake G (2011): Structural and elastic properties of $CaGeO_3$ perovskite at high pressures, Physics of Earth and Planetary Interiors, 189, 151-156.
53. Mookherjee M, Nakajima Y, Steinle-Neumann G, Glazyrin K, **Wu X**, Dubrovinsky L, McCammon C, Chumakov A (2011): High-pressure behavior of iron carbide (Fe7C3) at inner core conditions, Journal of Geophysical Research, 116, B04201.
52. Zhang Q, **Wu X***, and Shan Q (2011): In situ high-pressure X-ray diffraction experiments and ab initio calculations of $Co_2P$, Chinese Physics B, 20, 066101:1-6.
51. Zhang Q, Yang J, **Wu X***, and Qin S (2011): Phase stability and elasticity of $Sc_2O_3$ at high pressure, The European Physical Journal B, 84, 11-16.
50. Zhai S M, Xue W H, Lin C C, **Wu X**, Ito E (2011): Raman spectra and X-ray diffraction of tuite at various temperatures, Physics and Chemistry of Minerals, 38: 639-646.
49. Liu Y X, Qin S, **Wu X**, Jiang J Z, Kikegawa T, Shi G H (2011): High pressure X-ray diffraction study of $SrMnO_3$ perovskite, Chinese Physics C, 35, 514-518.
48. 杨晶,顾婷婷,朱峰,**巫翔***,秦善,刘景,李晓东(2011): 冰晶石($Na_3AlF_6$)的高压研究:同步辐射 X 射线衍射和第一性原理计算，核技术，34(6), 406-410
47. 杨晶,**巫翔***,秦善(2011): $(Fe_{0.03}Ni_{0.97})_8(Si_{0.79}P_{0.21})_3$ 的等温状态方程研究，高压物理学报，

25(3), 275-280

**2010 年**

46. **Wu X***, Steinle-Neumann G, Narygina O, McCammon C, and Dubrovinsky L (2010) In situ high-pressure study of $LiNbO_3$-type $FeTiO_3$: X-ray diffraction and Mössbauer spectroscopy, High Pressure Research, 30, 395- 405.
45. Zhai S M and **Wu X** (2010): X-ray diffraction study of β-$Ca_3(PO_4)_2$ at high pressure, Solid State Communications, 150, 443-445.
44. Zhai S M, **Wu X** and Ito E (2010): High-pressure Raman spectra of tuite, γ-$Ca_3(PO_4)_2$ , Journal of Raman Spectroscopy, 41, 1011-1013.
43. **Wu X***, Holbig E, and Steinle-Neumann G (2010) Structural stability of $TiO_2$ at high pressure in density-functional theory based calculations, Journal of Physics: Condensed Matter, 22, 295501.
42. Ovsyannikov S V, **Wu X**, Shchennikov V V, Karkin A E, Dubrovinskyaia N, Garbarino G, and Dubrovinsky L (2010) Structural stability of a golden semiconducting orthorhombic polymorph of $Ti_2O_3$ under high pressures and high temperatures, Journal of Physics: Condensed Matter, 22, 375402.
41. **Wu X***, Qin S, Dubrovinsky L (2010) Structural characterization of the $FeTiO_3$-$MnTiO_3$ solid solution, Journal of Solid State Chemistry, 183, 2483-2489.
40. **Wu X***, and Qin S (2010) First-principles calculations of the structural stability of $Fe_2P$, Journal of Physics: Conference Series, 215, 012110.
39. McCammon C, Dubrovinsky L, Narygina O, Kantor I, **Wu X**, Glazyrin K, I. Sergueev, Chumakov A I (2010) Low-Spin $Fe^{2+}$ in silicate perovskite and a possible layer at the base of the lower mantle, Physics of the Earth and Planetary Interiors, 180, 215-221.

**2009 年**

38. **Wu X***, Steinle-Neumann G, Qin S, Kanzaki M, and Dubrovinsky L (2009): Pressure-induced phase transitions of $AX_2$-type iron pnictides: an ab initio study, Journal of Physics: condensed matter, 21, 185403
37. **Wu X***, Steinle-Neumann G, Narygina O, Kantor I., McCammon C, Prakapenka V, Swamy V, and Dubrovinsky L (2009): High-pressure behavior of perovskite: $FeTiO_3$ dissociation into $(Fe_{1-\delta},Ti_\delta)O$ and $Fe_{1+\delta}Ti_{2-\delta}O_5$, Physical Review Letters, 103, 065503
36. **Wu X***, and Steinle-Neumann G (2009): Phase stability and elasticity of $ScAlO_3$ at high pressure, Geochimica et Cosmochimica Acta,73, A1454
35. Zhang H, **Wu X**, Nickel K G, Chen J, and Presser V (2009): High-pressure powder x-ray diffraction experiments and ab initio calculcation of $Ti_3AlC_2$, Journal of Applied Physics, 106, 013519
34. Dubrovinsky L, El Goresy A, Gillet P, **Wu X**, and Simionivici A (2009): A novel natural shock-induced high-pressure polymorph of $FeTiO_3$ ilmenite with the Li-Niobate structure from the Ries Crater, Germany, Meteorites & Planetary Science, 44, A64
33. Narygina O, Mattesini M, Kantor I, Pascarelli S, **Wu X**, Aquilanti G, McCammon C and Dubrovinsky L (2009): High-pressure experimental and computational XANES studies $(Mg,Fe)(Si,Al)O_3$ perovskite and (Mg,Fe)O ferropericlase as in the Earth's lower mantle, Physical Review B, 79, 174115

32. Narygina O, Kantor I, **Wu X**, Pascarelli S, Aquilanti G, McCammon C and Dubrovinsky L (2009): XANES study of spin crossover in Fe-bearing silicate perovskite, Phase Transition, 82, 336-343
31. **Wu X***, Steinle-Neumann G, Narygina O, Kantor I., McCammon C, Pascarelli S, Aquilanti G, Prakapenka V, and Dubrovinsky L (2009): Iron oxidation state of $FeTiO_3$ under high pressure. Physical Review B, 79, 094106
30. **Wu X***, Kanzaki M, Qin S, Steinle-Neumann G, and Dubrovinsky L (2009): Structural study of $FeP_2$ at high pressure, High Pressure Research, 29, 235-244

**2008 年以前**

29. Chen D L, Zhong J, **Wu X**, Wu Z Y, Mironova-Ulmane N, Kuzmin A, and Marcelli A(2008): Oxygen K-edge XANES investigation of $Ni_cMg_{1-c}O$ solid solutions, Spectrochimica Acta Part A, 70, 458-461
28. **Wu X** and Wu Z Y (2006): Theoretical calculations of the high-pressure phases of $ZnF_2$ and $CdF_2$, The European Physical Journal B, 50, 521-526
27. **Wu X**, Qin S and Wu Z Y (2006): First-principles study of structural stabilities, electronic and optical properties of $CaF_2$ under high pressure, Physical Review B, 73, 134103:1-8
26. **Wu X**, Qin S and Wu Z Y (2006): GGA calculations of the high-pressure behavior of $YAlO_3$ perovskite, Journal of Physics: Condensed Matter, 18, 3907-3916
25. **Wu X**, Wu Z Y, Guo L, Liu C, Liu J, and Li X D (2005): Pressure-induced phase transformation in controlled shape ZnO nanorods, Solid State Communication, 135, 780-784
24. **Wu X**, Dong Y H, Qin S, Abbas M I, Wu Z Y (2005): First-principles study of pressure-induced phase transition in $CaTiO_3$, Solid State Communication, 136, 416-420
23. Ibrahim K, Qian H J, **Wu X**, Abbas M I, and Wang J O et al. (2004): O 2p hole-assisted electronic processes in the $Pr_{1-x}Sr_xMnO_3$ (x = 0.0, 0.3) system, Physical Review B, 70, 224433:1-9
22. Qin S, **Wu X**, Liu J, Liu J, Wu Z Y, Li X D, and Lu A H (2003): Compressibility of Epidote up to 20 GPa at 298 K, Chinese Physics Letters, 20(7), 1172-1174
21. **Wu X**, Qin S, Wu Z Y, Dong Y H, Liu J, and Li X D (2003): Perovskites (Pbnm) structures transformations at high pressure, High Energy Physics and Nuclear Physics, 27(supp), 72-76
20. Qin S, **Wu X**, Seifert F, and Becerro A I (2002): Micro-Raman Study of Perovskite in the $CaTiO_3$-$SrTiO_3$ System, Journal of the Chemical Society. Dalton Transactions, 19, 3751-3755
19. 马陈燕, 崔明启, 张凌云, **巫翔**, 周克谨, 吴自玉, 陈兴. $(Fe_{1-x}Ni_x)_2P$ 电子结构与磁学特性的 X 射线近边吸收谱研究, 物理学报, 2008,57(6), 3868-3874
18. 李海铭, **巫翔**, 李炯, 陈栋梁, 储旺盛, 吴自玉. 高压下 LiF 和 NaF 的结构稳定性及其电子和光学性质的第一性原理研究, 物理学报, 2007, 56(12), 7201-7206
17. 李玉娟,**巫翔**,秦善,吴自玉. β-$MnO_2$ 高压相的从头计算模拟, 高压物理学报, 2006,20(3), 285-290
16. 李海建,秦善,刘景,李晓东,**巫翔**.方钠石的原位高压 X 射线研究.岩石矿物学杂志,2006,25(4):323-326
15. 祝向平,秦善,刘景,**巫翔**,李晓东,吴忠华.榍石的高压结构研究.矿物岩石,2006,26(3):6-11
14. 陈美华,陈征,狄敬如,路风香,**巫翔**.Ⅰa 型褐色金刚石结构缺陷的同步辐射白光形貌特征.地球科学-中国地质大学学报,2005,30(2):187-190
13. 秦善,刘景,祝向平,**巫翔**,李晓东.同步辐射与高压矿物学研究.地学前缘,2005,12(1):115-122

13. **巫翔**,秦善,吴自玉.从头计算在矿物压致相变研究中的应用.地质科技情报,2005,24(3):25-30
12. 龚平,陈涛,**巫翔**.湖南含籽晶天然金刚石的同步辐射 X 射线衍射形貌像研究.地质科技情报,2005,24(3):31-34
11. 奎热西·依布拉欣,钱海杰,买买提明·阿巴斯,苏润,**巫翔**等.$Pr_{1-x}Sr_xMnO_3$ 体系中 O2P 空穴参与的 O1s 近边吸收谱.核技术,2005,28(3):183-186
10. 王嘉鸥,奎热西,**巫翔**等.$SrTi_{1-x}Ru_xO_3$ 系列类钙钛矿结构氧化物的电子结构研究.高能物理与核物理.2005:47-50
9. 陈涛,**巫翔**,亓利剑,王河锦.人造金刚石晶体缺陷的同步辐射 X 射线衍射形貌像浅析.人工晶体学报,2005,34(1):33-37
8. **巫翔**,秦善,吴自玉,董宇辉,刘景,李晓东.钙钛矿 $CaTiO_3$ 的超高压结构研究.物理学报,2004,53(6):1967-1971
7. 祝向平,秦善,韩宝福,刘景,李晓东,**巫翔**.钛闪石的高压结构及其地质意义.岩石学报,2004,20(6):1456-1460
6. 李海建,秦善,祝向平,刘景,李晓东,**巫翔**,吴自玉.电气石的原位高压 X 射线衍射研究.核技术,2004,27(12):919-922
5. **巫翔**,秦善,李晓东,刘景,吴自玉.天然矿物硬玉($NaAlSi_2O_6$)的压致相变研究.核技术,2004,27(12):923-925
4. 陈涛,**巫翔**.合成金刚石的同步辐射劳埃形貌相研究.宝石和宝石学杂志,2004,6(1):13-16
3. **巫翔**,吴自玉,田玉莲等.同步辐射 X 射线形貌术在宝石学中的应用.宝石和宝石学杂志,2003,5(3):15-18
2. **巫翔**,周蜜.山东褐色蓝宝石的宝石学特征.珠宝科技,2001,(4):31-33
1. 秦善,鲁安怀,**巫翔**.$Ca_{1-x}Sr_xTiO_3$($0\leq x\leq 1$)体系粉晶 X 射线研究.北京大学学报(自然科学版),2001,37(6):827-831