



(2007—2010) (已结题)

4) 2006年国家自然科学基金面上项目1项(40672033), 项目名称“酸性条件下石英溶解分子机理的计算量子矿物学研究”: (2006—2009) (已结题)

5) 中国科学院“百人计划”项目1项(引进国外杰出人才类), 项目名称“稳定同位素平衡分馏的量子化学计算”: (2006—2010) (已结题) 终期评估优秀

6) 1997年国家自然科学基金青年基金项目1项(49601012), 项目名称“伊利石钾素释放的量子化学静电势计算研究”: (1997—2000) (已结题)

7) 1993年贵州省自然科学基金面上项目1项, 项目名称“金沙伊利石的高温性质及农业应用的可行性”: (1993-1995) (已结题)

#### 专家类别:

中国科学院百人计划入选者

#### 职务:

#### 社会任职:

? 中国矿物岩石地球化学学会理事(2009—2014)? 中国矿物岩石地球化学学会 矿物物理及矿物结构专业委员会委员、实验矿物岩石地球化学专业委员会委员、工艺矿物学专业委员会委员(2009—2014)? 矿床地球化学国家重点实验室学术委员会委员

#### 获奖及荣誉:

1) 中国矿物岩石及地球化学学会第十一届侯德封青年科学家奖(2006年)

2) 中国科学院“百人计划”终期评估优秀完成者(2010年)

3) 第四届贵州省优秀科技工作者(2011年)

#### 代表论著:

代表性SCI论文(作为第一或通讯作者):

Li, X.F. and Liu, Y.\* (2011) Equilibrium Se isotope fractionation parameters: A first-principles study. *Earth and Planetary Science Letters*, 304, 113-120.

Liu Q., Tossell J. A. and Liu, Y.\* (2010) On the proper use of the Bigeleisen-Mayer equation and corrections to it in the calculation of isotopic fractionation equilibrium constants. *Geochimica et Cosmochimica Acta*, 74, 6965-6983.

Li, X.F. and Liu, Y.\* (2010) First-principles study of Ge isotope fractionation during adsorption onto Fe(III)-oxyhydroxides surfaces. *Chemical Geology*, 278, 15-22.

Li, X.F., Zhao, H., Tang, M. and Liu, Y.\* (2009) Theoretical prediction for several important equilibrium Ge isotope fractionation factors and the geological implication. *Earth and Planetary Science Letters*, 287, 1-11.

Liu, Y., Olsen, A. A. and Rimstidt, J. D. (2006) Mechanism for the dissolution of olivine series minerals in acidic solutions. *American Mineralogist*, 91, 455-458.

Liu, Y. and Tossell, J.A. (2005) *Ab initio* molecular orbital calculations for boron isotope fractionations on boric acids and borates. *Geochimica et Cosmochimica Acta*, 69, 3995-4006.

Liu, Y., Nekvasil, H. and Tossell, J.A. (2005) Explaining the effects of T-O-T bond angles on NMR chemical shifts in aluminosilicates: A natural bonding orbital (NBO) analysis. *Journal of Physical Chemistry A*, 109, 3060-3066.

Liu, Y., Tossell, J. A. and Nekvasil, H. (2004) A theoretical study of structural factors correlated with  $^{23}\text{Na}$  NMR parameters. *American Mineralogist*, 89, 1314-1322.

Liu, Y. and Tossell, J. (2003) The possible Al-F bonding in F-bearing aluminosilicate glasses: from *ab initio*  $^{19}\text{F}$  NMR calculation study. *Journal of Physical Chemistry B*, 107, 11280-11289.

Liu, Y. Long, H. B. and Nekvasil, H. (2002) Water dissolution in albite melts: constraints from *ab initio* NMR calculations. *Geochimica et Cosmochimica Acta*, 66, 4149-4163.

Liu, Y. and Nekvasil, H. (2002) Si-F bonding in aluminosilicate glasses - inferences from *ab initio* NMR calculations. *American Mineralogist* 87, 339-346.

Liu, Y. and Nekvasil, H. (2001) *Ab initio* studies of possible fluorine-bearing four- and five- coordinated Al species in aluminosilicate glasses. *American Mineralogist* 86, 491-497.

#### 国际会议口头报告

**Yun Liu**, Qi Liu and John A. Tossell. Equilibrium isotope fractionation calculation beyond harmonic level. 2011 ACS National Spring Meeting, Anaheim, CA. (Invited talk 40 minutes)

**Yun Liu** and Huiming Bao. Theoretical determination of O and S isotope fractionations between gypsum and aqueous sulfate. 2009 American Geophysical Union Fall meeting, EOS, Transactions, 90(52), B22B-08. **(talk)**

**Yun Liu** and Xiaobin Cao. Re-thinking of the isotope mass-independent fractionation (MIF) definition. 2009 Swiss 19th Annual V.M. Goldschmidt Conference. (talk)

**Yun Liu.** Theoretical study on the mechanism of the removal of Mo from seawater in oxic environment. 2008 Canada 18th Annual V.M. Goldschmidt Conference. (talk)

**Yun Liu** and Mao Tang. Iron isotopic fractionations between species in solution – from ab initio quantum chemistry calculations. 2006 Australia 16th Annual V.M. Goldschmidt Conference. (talk)

**Yun Liu,** Mao Tang and John A. Tossell. The boron isotopic paleo-pH indicator- a theoretical re-evaluation. Beijing 7th International Symposium on Environmental Geochemistry. (talk)

**Yun Liu,** J. D. Rimstidt and G.V. Gibbs, A Theoretical Study on the Dissolution Mechanisms of Forsterite. 2004 American Geophysical Union Fall meeting. (talk)

**Yun Liu** and John Tossell, Ab initio molecular orbital calculations for boron isotope fractionations on boron acids and borates. 2003 American Geophysical Union Fall meeting, EOS, Transactions, F1634. (talk)

**Yun Liu** and Hanna Nekvasil, Water dissolution in albite melts: constraints from ab initio NMR calculations. 2002 Glass & Optical Materials Division Fall Meeting of the American Ceramic Society. (talk)

**Yun Liu** and Hanna Nekvasil, Is there Si-F bonding in aluminosilicate glasses? Inferences from ab initio NMR calculations. 2000 American Geophysical Union Fall meeting, EOS, Transactions, F1328. (talk)

