Tian Qin

Education

Ph.D. in Earth Sciences, minor in Chemistry
University of Minnesota – Twin Cities

May 2019
Minneapolis, MN, USA

Master of Science in GeophysicsJun 2014University of Science and Technology of China (USTC)Hefei, Anhui, China

Bachelor of Science in GeologyJun 2011Nanjing UniversityNanjing, Jiangsu, China

Skills

Programming
 Machine Learning
 Software
 Python3, MATLAB/Octave, Bash Shell, Fortran
 Numpy/Scipy/Matplotlib/Pandas/; Logistic Regression, Neural Networks
 LaTeX/MS office/Markdown/PyCharm/Git/Vim/VS Code/Quantum Espresso/Gaussian

Research Experience

Research Assistant, University of Minnesota, MN

Jun 2016 - May 2019

- Developed qha for quasi-harmonic free energy calculation in Python3
 - o Deal with systems with single/multi-configuration
 - o Easy to prepare the input file
 - Use ~10% running time compared to the old Fortran code
- o Investigated the structures and stability field of hydrous defects in olivine using quantum chemistry calculations
 - o Find 16 stable defects configurations out of 200+ possible configurations
 - o Determine the effect of configurational entropy on the stability of defects
- o Investigated the Fe isotope fractionation behavior in the lower mantle using quantum chemistry calculations

Visiting Student, Columbia University, NY

Sep 2017 - Aug 2018

- o Investigated the Fe/Si isotope fractionation behavior in the lower mantle and core
- o Led group of 6 junior graduate students to calculate the properties of Fe and AlOOH

Research Assistant, USTC, Hefei, China

Sep 2011 – Jun 2014

- o Investigated the Si and O isotope fractionation in crust using ab initio calculations
- o Investigated the V isotope fractionation in the solutions using ab initio calculations
- o Investigated the concentration effect of Ca isotope in CPX and OPX

Teaching Experience

Lab Instructor, University of Minnesota, MN

Sep 2014 – May 2016

- Guide about 40 students to work on the Lab of "Earth and its Environment."
- o Respond to questions in an engaging manner

Resource Instructor, University of Minnesota, MN

Summer 2016, 2017

o Teach new international graduate students the teaching assistant system in the UMN

Publications

Published (* corresponding author)

- 1. Zhang, Z*., Qin, T., Pommier, A., Hirschmann, M.M*., 2019. Carbon storage in Fe-Ni-S liquids in the deep upper mantle and its relation to diamond and Fe-Ni alloy precipitation. Earth and Planetary Science Letters 520, 164–174. https://doi.org/10.1016/j.epsl.2019.05.039
- 2. **Qin, T.,** Zhang, Q., Wentzcovitch, R*., Umemoto, K., qha: A Python package for quasiharmonic free energy calculation for multi-configuration systems, Computer Physics Communications (2018), https://doi.org/10.1016/j.cpc.2018.11.003.
- 3. **Qin, T.,** Wentzcovitch, R.*., Umemoto, K., Hirschmann, M. M. & Kohlstedt, D. L. Ab initio study of water speciation in forsterite: importance of the entropic effect. Am. Mineral. (2018). doi:10.2138/am-2018-6262
- 4. Wang, W., **Qin, T.,** Zhou, C., Huang, S., Wu, Z*., Huang, F*., 2017. Concentration effect on equilibrium fractionation of Mg-Ca isotopes in carbonate minerals: insights from first-principles calculations. Geochim. Cosmochim. Acta. http://dx.doi.org/10.1016/j.gca.2017.03.023
- 5. Wang, W., Zhou, C., **Qin, T.**, Kang, J.-T., Huang, S., Wu, Z*., Huang, F., 2017. Effect of Ca content on equilibrium Ca isotope fractionation between orthopyroxene and clinopyroxene. Geochim. Cosmochim. Acta 219, 44–56. https://doi.org/10.1016/j.gca.2017.09.022
- 6. **Qin, T.**, Wu, F., Wu, Z*., Huang, F*., 2016. First-principles calculations of equilibrium fractionation of O and Si isotopes in quartz, albite, anorthite, and zircon. Contrib. to Mineral. Petrol. 171, 91. doi:10.1007/s00410-016-1303-3
- 7. Wu, F*., Qin, T*., Li, X., Liu, Y., Huang, J.-H., Wu, Z., Huang, F., 2015. First-principles investigation of vanadium isotope fractionation in solution and during adsorption. Earth Planet. Sci. Lett. 426, 216–224. doi:10.1016/j.epsl.2015.06.048
- 8. Feng, C., **Qin, T.,** Huang, S., Wu, Z*., Huang, F*., 2014. First-principles investigations of equilibrium calcium isotope fractionation between clinopyroxene and Ca-doped orthopyroxene. Geochim. Cosmochim. Acta 143, 132–142. doi:10.1016/j.gca.2014.06.002

In preparation

- 1. **Qin, T.**, Marcondes, M., Wentzcovitch, R*., Shukla, G., Wu, Z., Iron isotope fractionation in the core formation.
- 2. **Qin, T.**, Marcondes, M., Wentzcovitch, R*., Silicon isotope fractionation between silicate minerals and FeSi alloy.

Selected Talks/Posters

- 1. Qin, T., Wentzcovitch, R., Marcondes, and M., Shukla, G., Ab initio study of iron isotope fractionation during Earth's core-mantle segregation, 2019 APS March Meeting, Oral presentation.
- 2. Qin, T., Marcondes, M., Shukla, G., and Wentzcovitch, R., Iron isotope fractionation during Earth's core-mantle segregation. Fall 2018 AGU Abstract and Poster.
- 3. Zhang., Qi., Qin, T., Wentzcovitch, R., qha: A Python package for quasi-harmonic free energy calculation for multi-configuration systems., Fall 2018 AGU Abstract.
- 4. Qin, T., Umemoto, K., Wentzcovitch, R., Hirschmann, M., and Kohlstedt, D., "Ab initio study of hydrous Mg- and Sivacancies in forsterite: their stability and IR signatures" Fall 2016, AGU Abstract and Poster.
- 5. Qin, T., Wu, F., Wu, F., and Huang, F., First-principles investigation of equilibrium isotopic fractionation of Si and O isotope among quartz, albite, anorthite, orthoenstatite, clinoenstatite, olivine and zircon. Fall 2013 *AGU*, Abstract.

Honors and Awards

- o Thomas Andrews Fellowship, Department of Earth Sciences, University of Minnesota (2018)
- o Francis Gibson Fellowship, Department of Earth Sciences, University of Minnesota (2016)

Service

Reviewer of peer-reviewed journal: GCA (Geochim. Cosmochim. Acta)