
Qiang Zhu

ESS 255, Stony Brook Univ, Stony Brook, NY, 11794-2100 Tel: 631-879-8862
Email: qiazhu@ic.sunysb.edu

Education Background

◆ Undergraduate

B.S, Materials Science and Engineering, *Beihang University*, July. 2007

◆ Postgraduate

Materials Science and Engineering, *Beihang University*, Sept. 2007 – July, 2009

◆ PhD

Geosciences, *State University of New York at Stony Brook*, Sept. 2009 – present

Research Interest

Computational Materials & Minerals Science

1. Methodology development: **Ab-initio simulation, Molecular dynamics, Evolutionary algorithms**
2. Application: **Theoretical prediction for bulk, molecule & surface structures**

Research Experience

- ◆ Sept. 2006 – July 2009, **Classical & ab-initio molecular dynamic simulation of amorphous materials**
 - Dynamics of SiO₂ glasses based on BKS/Morse potential (**Potential development, Rapid quench algorithm**)
 - Models to describe amorphous Si-B-C-N network (**Rapid quench algorithm, Amorphous structure, Bonding analysis**)
 - Simulate the crystal phase transition of Si-C-N in high pressure
- ◆ Sept. 2009 – present, **Evolutionary algorithm used for structural prediction: methodology and application:**
 - Method development for *molecular crystal* structure prediction
 - Method development for *surfaces structure* prediction
 - Ab initio search for novel polymorphs for pure *carbon* and *carbon compounds*
 - Organic molecular crystal prediction on *glycine*
 - Webmaster of USPEX download page

Teaching Experience

- ◆ Sept. 2009 – June. 2010, **Teaching Assistant in Geosciences Dept at Stony Brook University**

Additional Technical Experience

- ✧ Unix system Administrator (2007-present).
 - *Beihang Univ*, Department of Materials Science and Engineering. Prof. Zhang group (2007-2009). Setup and administration of computer clusters for ab-initio quantum calculations of materials.
 - *Stony Brook Univ*, Department of Geosciences. Prof. A. R. Oganov's group (2009 - present). Maintenance of computer clusters
 - *Stony Brook Univ*, Department of Geosciences. Prof. A. R. Oganov's group (2009 - present). The author and webmaster of USPEX download webpage.

Participation in Conference

- ✧ Proceedings of 06th International Material Week, (Beijing, China, 2006)
- ✧ 6th International Conference on Materials Processing for Properties and Performance, (Beijing, China, 2007)
- ✧ Theoretical and computational methods in mineral physics: applications to geophysics (Berkeley, CA, US, 2009)
- ✧ American Physical Society March meeting (Dallas, TX, US, 2011)

Publications

- ✧ Fanwei Zhang, **Qiang Zhu**, etc, *Molecular Dynamics Study of Diffusion Behavior in Amorphous Silica with Hydroxyl Group*, [J]Key Engr Mat. Vols.368-372(2008) 1677-79
- ✧ **Qiang Zhu**, etc, *A Novel Approach for the Effective Thermal Conductivity of Porous Ceramics*, [J] Chin J of Aero. Vol. 19(2006), S244-47
- ✧ **Qiang Zhu**, Oganov A.R., Salvado M., Pertierra P., Lyakhov A.O. (2011). Denser than diamond: ab initio search for superdense carbon allotropes. *Phys. Rev. B*, in press.

Computational Skills

- ✧ Environment: Linux, Unix, MS-DOS, Windows
- ✧ Languages: C, C++, Fortran, Matlab, Perl, Html
- ✧ Software & Codes: USPEX, CPMD, VASP, ANSYS, DL_POLY, Materials Studio, GULP, DMACRYS
- ✧ Addition: Linux Cluster Management, Web-page Management