# QIANG ZHU

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## EDUCATION

**Ph.D.**, Geosciences, *State University of New York at Stony Brook* (2009-2013)

**B.S.**, Materials Science and Engineering, *Beihang University* (2003-2007)

## RESEARCH EXPERIENCE

**Assistant Professor**, University of Nevada, Las Vegas, since Oct 2016

**Research Assistant Professor**, Stony Brook University, Feb 2014 - Sept 2016

**Research Associate**, Stony Brook University, Feb 2013 - Feb 2014

**Research Assistant**, Stony Brook University, Aug 2009 - Feb 2013

- Organic crystal polymorphism
- Materials under extreme conditions
- Materials defects
- High-throughput materials design
- Phase Transition Mechanisms

## TEACHING EXPERIENCE

**Lecturer** in *Statistic Mechanics* undergrad/grad, 2018 spring
**Lecturer** in *Computational Physics* undergrad, 2017 fall
**Lecturer** in *Thermodynamics* undergrad/grad, 2017 spring
**Lecturer and tutor** in a series of international worshops (France, 2011/2015; China, 2011/2013/2015; Switzerland, 2012; USA, 2012; Isarel, 2013; Canada, 2014; India, 2015; Italy, 2016)
**Co-lecturer** in *Structure and Properties of Materials* (graduate), 2014 fall
**Co-lecturer** in *Topics in Mineralogy and Crystallography* (undergrad), 2013 spring
Teaching Assistant in *Environmental Geology* and *The Earth* (undergrad), 2009-2010

## GRANTS, AWARDS, ACTIVITIES

APS-SCCM student fellowship, 2013

Qianjiang Scholarship, Beihang University (2008)
President's Award for Distinguished Doctoral Students, Stony Brook University (2013)

**Editorial Member** of Scientific Reports (since 2015 June)
**Reviewer** for *Nature Communication, J. Am. Chem. Soc., J. Mater. Chem. A., npj computational materials, Scientific Reports, App. Phys. Lett., Phys. Chem. Chem. Phys., Euro. Phys. Lett., Solid State Comm., J. Mater. Chem. C, J. Non-Crystalline Solids, Chem. Mater., Acta Cryst*

## INVITED TALKS

American Chemical Soeciety March meeting, San Diego, CA, 2012
Society for Industrial and Applied Mathematics, Minneapolis, MN, 2012
American Geophysic Union fall meeting, San Francisco, CA, 2012
Provost's lecture series, Stony Brook, NY, 2013 (**Highest honor for Doctoral students**)
Workshop on Theoretical Tools for Catalyst Design, Beijing, 2013 (**plenary talk**)

American Crystallographic Association, Honolulu, HI, 2013
All Oxides Photovoltaics Workshop, Jerusalem, Israel, 2013 (**plenary talk**)
23rd IUCr Congress, Montreal, Canada, 2014
Invited seminar, MIT Cambridge, MA, 2014
Invited seminar, Skoltech, Moscow, Russia, 2014
International Conference on Chemical Bonding, Kauai, HI, 2015
Blind Test Workshop for Organic Crystal Structure Prediction, Cambridge, UK, 2015
Lunar and Planetary Institute Seminar Series, Houston, TX, 2017
Genomic Approaches to Accelerated Materials Innovation, MRS conference, 2017
Shanghai International Crystallographic School working with Bilbao Crystallographic Server, 2017

## PUBLICATIONS

### PATENTS

1. A. R. Oganov, A. O. Lyakhov, **Q. Zhu**, Method for predicting optimized crystal structures, US Patent App. 13/534,861 purchased by SONY
2. A. R. Oganov,**Q. Zhu**, Materials for storage of flourine and chlorine, US Patent App. 61/971,763

### BOOK CHAPTERS

3. **Q. Zhu***, A. R. Oganov, Q-F. Zeng, X-F. Zhou, Structure Prediction and its application in Computational Materials Design. *Chemical Modelling* Royal Society of Chemistry (2016) DOI: 10.1039/9781782622703-00219
4. **Q. Zhu***, A. R. Oganov, X-F. Zhou, Crystal structure prediction and its application in Earth and Materials Sciences. *Topics in Current Chemistry - Prediction and Calculation of Crystal Structures: Methods and Applications* (Eds. Atahan-Evrenk/Aspuru-Guzik) Springer Series (2014) DOI: 10.1007/128_2013_508
5. A. R. Oganov, A. O. Lyakhov, **Q. Zhu**, Theory of Superhard Materials. *Comprehensive Hard Materials.* 3, 59-79 (2014)

### PEER REVIEW PAPERS **(40+ papers in total, 1800+ citations since 2010)**

6. **Q. Zhu***, *et al.*, Stability of xenon oxides at high pressures. Nature Chemistry, 5(2013), 61-65
7. **Q. Zhu**, A. Samanta, B-X, Li, R.E. Rudd, T. Frolov, Predicting phase behavior of grain boundaries with evolutionary search and machine learning. Nature Communication, 9(2018), 467
8. A. G. Shtukenberg, **Q. Zhu***, *et al* Powder diffraction and crystal structure prediction identify four new coumarin polymorphs. Chemical Science, 8(2017) 4926-4940
9. W. Xu, **Q. Zhu***, Hu CT. Structure of Glycine Dihydrate: Its implications to Crystallization of Glycine from Solution and Modification of Glycine in Space. Angew. Chem. Int. Ed., 129(2017), 2062-2066
10. **Q. Zhu**, *et al.*, Resorcinol Crystallization from the Melt: A New Ambient Phase and New Riddles. J. Am. Chem. Soc., 138(2016), 4881-4889
11. W. Zhang, A. R. Oganov, A. Goncharov, **Q. Zhu**, *et al.*, Unexpected stable stoichiometries of sodium chlorides. Science, 342(2013), 1502-1505
12. X. Dong, A. R. Oganov, A. Goncharov, E. Stavrou, S. Lobanov, G. Saleh, G. Qian, **Q Zhu**, *et al.* A stable compound of helium and sodium at high pressure. Nature Chemistry, 9(2017), 440-445
13. V. Sharma, C. Wang, R. Lorenzini, R. Ma, **Q Zhu**, *et al.* Rational Design of All-Organic Polymer Dielectrics. Nature Communications, 5(2014), 4845
14. J Yang, CT Hu, X Zhu, **Q Zhu**, MD Ward, B Kahr, DDT Polymorphism and the Lethality of Crystal Forms. Angewandte Chemie, 129(2017), 10299-10303
15. Q. Wang, A. R. Oganov, **Q Zhu**, X-F Zhou, New Reconstructions of the (110) Surface of Rutile TiO2 Predicted by an Evolutionary Method. Phys. Rev. Lett, 113(2014), 266101
16. X-F Zhou, A. R. Oganov, X Shao, **Q Zhu**, *et al.*, Unexpected Reconstruction of the alpha-Boron (111) Surface. Phys. Lett. Lett, 113(2014), 176101

17. X-F Zhou, X Dong, A. R. Oganov, **Q Zhu**, *et al.*, Semimetallic Two-Dimensional Boron Allotrope with Massless Dirac Fermions. Phys. Lett. Lett, 112(2014), 085502
18. C-H. Hu, A. R. Oganov, **Q. Zhu**, G-R. Qian, G. Frapper, A. O. Lyakhov, and H-Y. Zhou, Pressure-induced stabilization and insulator-superconductor transition of BH. Phys. Rev. Lett., 110(2013), 165504
19. X-F. Zhou, A. R. Oganov, G-R. Qian, **Q. Zhu**, First-Principles Determination of the Structure of Magnesium Borohydride. Phys. Rev. Lett., 109(2012), 245503
20. Z. Wang, X-F. Zhou, X. Zhang, **Q. Zhu**, H. Dong, M. Zhao, A. R. Oganov, Phagraphene: A Low-Energy Graphene Allotrope Composed of 5-6-7 Carbon Rings with Distorted Dirac Cones. Nano Letters, 15(2015), 6182-6186
21. A. G. Shtukenberg, C-T, Hu, Q. **Zhu Q***, et al, The Third Ambient Aspirin Polymorph. Cryst. Growth Des., 17(2017), 3562-3566
22. X. Meng, L. Wang, D. Liu, X. Wen **Q. Zhu***, W. A. Goddad, Q. An, Discovery of Fe2P-Type Ti(Zr/Hf)2O6 Photocatalysts toward Water Splitting. Chem. Mater., 10.1021/acs.chemmater.5b04256, 2016
23. **Q. Zhu***, A. R. Oganov, *et al.*, Generalized Evolutionary Metadynamics for Sampling the Energy Landscapes and its Applications. Phys. Rev. B, 92(2015), 024106
24. **Q. Zhu***, A. R. Oganov. Evolution of $CsF_n$ Compounds under High Pressure, Scientific Reports., 5(2015), 7875
25. **Q. Zhu***, V. Sharma, A. R. Oganov, R. Ramprasad. Predicting Polymeric Crystal Structures by Evolutionary Algorithms. J. Chem. Phys., 141(2014), 154102
26. **Q. Zhu***, Q. Zeng, A. R. Oganov, Systematic search for low-enthalpy $sp^3$ carbon allotropes using evolutionary metadynamics. Phys. Rev. B, 85(2012), 201407
27. **Q. Zhu***, A. R. Oganov, *et al.*, Denser than diamond: *Ab initio* search for superdense carbon allotropes, Phys. Rev. B, 83(2011), 193410
28. **Q. Zhu***, L. Li, A. R. Oganov, P. B. Allen, Evolutionary Method for Predicting Surface Reconstructions with Variable Stoichiometry. Phys. Rev. B, 87(2013), 195317
29. **Q. Zhu***, A. R. Oganov, A. O. Lyahkov, Novel stable Mg-O compounds under high pressure. Phys. Chem. Chem. Phys., 15(2013), 7696-7700
30. **Q. Zhu***, A. R. Oganov, A. O. Lyakhov, Evolutionary metadynamics: A novel method to predict crystal Structures. CrystEngComm, 14(2012), 3596-3601
31. **Q. Zhu***, A. R. Oganov, *et al.*, Constrained evolutionary algorithm for structure prediction of molecular crystals: methodology and applications. Acta Cryst. B, 68(2012), 215-226
32. **Q Zhu***, *et al.* Metastable host-guest structure of carbon. J. Superhard Mater., 36(2014), 246-256 The phase diagram and hardness of carbon nitrides
33. S. Wang, A. R. Oganov, G. Qian, **Q Zhu**, *et al.* Novel superhard B-C-O hases predicted from first principles. Phys. Chem. Chem. Phys., 18(2016), 1859-1863
34. S. Lobanov, **Q. Zhu**, *et al.*, Stable magnesium peroxide at high pressure. Scientific Report., 5(2015), 13582
35. H Dong, A. R. Oganov, **Q Zhu**, G. R. Qian. The phase diagram and hardness of carbon nitrides. Scientific Report, 5(2015), 9870
36. Y. Liu, A. R. Oganov, S. Wang, **Q. Zhu**, X. Dong, and G. Kresse, Prediction of new thermodynamically stable aluminum oxides. Scientific Report, 5(2015), 9518
37. G-R. Qian, A. O. Lyakhov, **Q Zhu**, *et al.* Novel Hydrogen Hydrate Structures under Pressure. Scientific Report, 4(2014), 5606
38. H Niu, X Chen, W Ren, **Q Zhu**, AR Oganov, D Li, Y Li, Variable-composition Structural Optimization and Experimental Verication of $MnB_3$ and $MnB_4$, Phys. Chem. Chem. Phys., 16(2014), 15866
39. Q. Zeng, J. Peng, A. R. Oganov, **Q Zhu**, *et al.* Prediction of stable hafnium carbides: their stoichiometries, mechanical properties, and electronic structure, Phys. Rev. B, 88(2013), 214107

40. Q. Zeng, A. R. Oganov, A. O. Lyakhov, C. Xie, X. Zhang, J. Zhang, **Q Zhu**, *et al.* Evolutionary search for new high-k dielectric materials: methodology and applications to hafnia-based oxides. Acta Cryst. C, 70(2013), 76-84
41. A. O. Lyahkov, A. R. Oganov, H. T. Stokes, **Q. Zhu**, New developments in evolutionary structure prediction algorithm USPEX. Comp. Phys. Comm., 184(2013), 1172-1182
42. S. E. Boulfelfel, **Q. Zhu**, A. R. Oganov, Novel $sp^3$-forms of carbon predicted by evolutionary metadynamics and analysis of their synthesizability using transition path sampling. J. Superhard Mater., 34(2012), 350-359
43. MMD Esfahani, **Q. Zhu**, et al. Novel magnesium borides and their superconductivity. Phys. Chem. Chem. Phys, 19(2017), 14486