

QIANG ZHU

Geosciences Dept., Stony Brook University, Stony Brook, NY 11794-2100, Phone: (631)-632-1449
Email: qiang.zhu@stonybrook.edu, Website: <http://uspex.stonybrook.edu/qzhu.html>

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

Research Assistant Professor, Stony Brook University, Feb 2014 - Present

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

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

- Chief developer of the USPEX code for crystal structure prediction (~ 2500 users).
- Organic crystal polymorphism
- Materials under extreme conditions
- 2D crystals and surfaces reconstructions
- Search and design of (in)organic materials with superior properties
- Phase Transition Mechanisms

TEACHING EXPERIENCE

Lecturer and tutor in a series of international workshops (France, 2011/2015; China, 2011/2013/2015; Switzerland, 2012; USA, 2012; Israel, 2013; Canada, 2014; India, 2015)

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

American Crystallographic Association travel grant, 2013

APS-SCCM student fellowship, 2013

Qianjiang Scholarship, Beihang University (2008)

President's Award for Distinguished Doctoral Students, Stony Brook University (2013)

Editor of Scientific Reports (since 2015 June)

Reviewer for *Scientific Reports*, *App. Phys. Lett.*, *Phys. Chem. Chem. Phys.*, *Euro. Phys. Lett.*, *Solid State Comm.*, *J. Mater. Chem. C*, *J. Non-Crystalline Solids*

INVITED TALKS

American Chemical Society March meeting, San Diego, CA, 2012

Society for Industrial and Applied Mathematics, Minneapolis, MN, 2012

American Geophysical 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

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 (31 papers in total, 12 first-authored, 780 citations since 2010)

6. **Q. Zhu***, *et al.*, Stability of xenon oxides at high pressures. *Nature Chemistry*, 5(2013), 61-65
7. **Q. Zhu**, *et al.*, Resorcinol Crystallization from the Melt: A New Ambient Phase and New Riddles. *J. Am. Chem. Soc.*, 138(2016), 4881-4889
8. W. Zhang, A. R. Oganov, A. Goncharov, **Q. Zhu**, *et al.*, Unexpected stable stoichiometries of sodium chlorides. *Science*, 342(2013), 1502-1505
9. V. Sharma, C. Wang, R. Lorenzini, R. Ma, **Q. Zhu**, *et al.* Rational Design of All-Organic Polymer Dielectrics. *Nature Communications*, 5(2014), 4845
10. 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. Lett. Lett*, 113(2014), 266101
11. 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
12. 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
13. 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
14. 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
15. 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*, (2015)
16. 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
17. **Q. Zhu***, A. R. Oganov, *et al.*, Generalized Evolutionary Metadynamics for Sampling the Energy Landscapes and its Applications. *Phys. Rev. B*, 92(2015), 024106
18. **Q. Zhu***, A. R. Oganov. Evolution of CsF_n Compounds under High Pressure, *Scientific Reports.*, 5(2015), 7875

19. **Q. Zhu***, V. Sharma, A. R. Oganov, R. Ramprasad. Predicting Polymeric Crystal Structures by Evolutionary Algorithms. *J. Chem. Phys.*, 141(2014), 154102
20. **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
21. **Q. Zhu***, A. R. Oganov, *et al.*, Denser than diamond: *Ab initio* search for superdense carbon allotropes, *Phys. Rev. B*, 83(2011), 193410
22. **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
23. **Q. Zhu***, A. R. Oganov, A. O. Lyakhov, Novel stable Mg-O compounds under high pressure. *Phys. Chem. Chem. Phys.*, 15(2013), 7696-7700
24. **Q. Zhu***, A. R. Oganov, A. O. Lyakhov, Evolutionary metadynamics: A novel method to predict crystal Structures. *CrystEngComm*, 14(2012), 3596-3601
25. **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
26. **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
27. S. Wang, A. R. Oganov, G. Qian, **Q. Zhu**, *et al.* Novel superhard B-C-O phases predicted from first principles. *Phys. Chem. Chem. Phys.*, 18(2016), 1859-1863
28. S. Lobanov, **Q. Zhu**, *et al.*, Stable magnesium peroxide at high pressure. *Scientific Report.*, 5(2015), 13582
29. H Dong, A. R. Oganov, **Q. Zhu**, G. R. Qian. The phase diagram and hardness of carbon nitrides. *Scientific Report*, 5(2015), 9870
30. 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
31. G-R. Qian, A. O. Lyakhov, **Q. Zhu**, *et al.* Novel Hydrogen Hydrate Structures under Pressure. *Scientific Report*, 4(2014), 5606
32. H Niu, X Chen, W Ren, **Q. Zhu**, A. R. Oganov, D Li, Y Li, Variable-composition Structural Optimization and Experimental Verification of MnB_3 and MnB_4 , *Phys. Chem. Chem. Phys.*, 16(2014), 15866
33. 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
34. 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
35. A. O. Lyakhov, A. R. Oganov, H. T. Stokes, **Q. Zhu**, New developments in evolutionary structure prediction algorithm USPEX. *Comp. Phys. Comm.*, 184(2013), 1172-1182
36. 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