

Tiange Bi, Ph.D.

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Earth and Planets Laboratory
Carnegie Institution for Science

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Post Secondary Education

- Sep. 2014 – Jun. 2020 **Ph.D. in Chemistry**
State University of New York at Buffalo, Buffalo, NY, USA
Dissertation Title: “Density Functional Theory (DFT) Studies of Hydrogen Rich Materials, Methylammonium Lead Bromide Perovskite and Silicon Dioxide under Pressure”
Supervisor: Professor Eva Zurek
- Jan. 2010 – Dec. 2013 **B.Sc. in Chemistry**
University of Central Arkansas, Conway, Arkansas, USA

Professional Experience

- Aug. 2021 – Current **Postdoctoral Fellow** Earth and Planets Laboratory of the Carnegie Institution for Science
- Sep. 2020 – Aug. 2021 **Postdoctoral Associate** Research Group of Dr. Eva Zurek, Department of Chemistry, State University of New York at Buffalo
- Feb. 2017 – June 2020 **Research Assistant** Research Group of Dr. Eva Zurek, Department of Chemistry, State University of New York at Buffalo
- Sep. 2014 – Jan. 2017 **Teaching Assistant** Department of Chemistry, State University of New York at Buffalo
- Jan. 2013 – May 2013 **Teaching Assistant** Department of Chemistry, University of Central Arkansas

Research Publications

Number of Citations = 195, Hirsch index (h) = 6 (Web of Science)

Number of Citations = 362, Hirsch index (h) = 8 (Google Scholar)

Bibliography

- 14** Bi, Tiange; Shamp, Andrew; Terpstra, Tyson; Hemley, R.; Zurek, Eva; “The Li–F–H Ternary System at High Pressures” *J. Chem. Phys.* **2021**, *154*, 124709.
- 13** Yan, Yan; Bi, Tiange; Geng, Nisha; Wang, Xiaoyu; Zurek, Eva; “A Metastable CaSH₃ Phase Composed of HS Honeycomb Sheets that is Superconducting Under Pressure” *J. Phys. Chem. Lett.* **2020**, *11*, 9629–9636.
- 12** Cui, Xiangyue; Hilleke, Katerina P.; Wang, Xiaoyu; Lu, Mingchun; Zhang, Miao; Zurek, Eva; Li, Wenjing; Zhang, Dandan; Yan, Yan; Bi, Tiange; “RbB₃Si₃: An Alkali Metal Borosilicide that is Metastable and Superconducting at 1 atm” *J. Phys. Chem. C* **2020**, *124*, 14826–14831.
- 11** Zhang, Dandan; Xu, Xuedi; Lu, Mingchun; Bi, Tiange; Tian, Yuanye; Zhang, Songbo; Yan, Yan; Du, Yonghui; Zhang, Miao; Gao, Lili; “Predicted Crystal Structures of Titanium Nitrides at High Pressures” *Comput. Mater. Sci.* **2020**, *180*, 109720.
- 10** Cui, Wenwen*; Bi, Tiange* (*Authors contributed equally to this work); Shi, Jingming; Li, Yinwei; Liu, Hanyu; Zurek, Eva; Hemley, Russell J.; “Route to High-*T_c* Superconductivity via CH₄-Intercalated H₃S Hydride Perovskites” *Phys. Rev. B* **2020**, *101*, 134504.

- 9 Geng, Nisha; **Bi, Tiange**; Zarifi, Niloofar; Yan, Yan; Zurek, Eva; “A First-Principles Exploration of Na_xS_y Binary Phases at 1 atm and Under Pressure” *Crystals* **2019**, 9, 441.
- 8 **Bi, Tiange**; Zarifi, Niloofar; Terpstra, Tyson; Zurek, Eva; “The Search for Superconductivity in High Pressure Hydrides”; in “Chemistry, Molecular Sciences and Chemical Engineering” In *Reference Module in Chemistry, Molecular Sciences and Chemical Engineering*, Reedijk, J., Ed.; Elsevier: 2019, (Invited Review).
- 7 Zurek, Eva; **Bi, Tiange**; “High-Temperature Superconductivity in Alkaline and Rare Earth Polyhydrides at High Pressure: A Theoretical Perspective” *J. Chem. Phys.* **2019**, 150, 050901. (Invited Review).
- 6 Fu, Zhongheng; **Bi, Tiange**; Zhang, Shihao; Chen, Shu; Zurek, Eva; Legut, Dominik; Germann, Timothy; Lookman, Turab; Zhang, Ruifeng; “Anchoring Effect of Distorted Octahedra on the Stability and Strength of Platinum Metal Pernitrides” *Phys. Rev. Mater.* **2019**, 3, 013603.
- 5 Zarifi, Niloofar; **Bi, Tiange**; Liu, Hanyu; Zurek, Eva; “Crystal Structures and Properties of Iron Hydrides at High Pressure” *J. Phys. Chem. C* **2018**, 122, 24262–24269.
- 4 Shelton, Hannah; **Bi, Tiange**; Zurek, Eva; Smith, Jesse; Dera, Przemyslaw; “The Ideal Crystal Structure of Cristobalite X-I: A Bridge in SiO_2 Densification” *J. Phys. Chem. C* **2018**, 122, 17437–17446.
- 3 **Bi, Tiange**; Miller, Daniel P.; Shamp, Andrew; Zurek, Eva; “Superconducting Phases of Phosphorus Hydride Under Pressure: Stabilization by Mobile Molecular Hydrogen” *Angew. Chem. Int. Ed.* **2017**, 56, 10192–10195.
- 2 Zhang, Rong; Cai, Weizhao; **Bi, Tiange**; Zarifi, Niloofar; Terpstra, Tyson; Zhang, Chuang; Vardeny, Z. Vally; Zurek, Eva; Deemyad, Shanti; “Effects of Non-Hydrostatic Stress on Structural and Optoelectronic Properties of Methylammonium Lead Bromide Perovskite” *J. Phys. Chem. Lett.* **2017**, 8, 3457–3465.
- 1 Shamp, Andrew; Terpstra, Tyson; **Bi, Tiange**; Falls, Zackary; Avery, Patrick; Zurek, Eva; “Decomposition Products of Phosphine Under Pressure: PH_2 Stable and Superconducting?” *J. Am. Chem. Soc.* **2016**, 138, 1884–1892.

Awards

- 2019 **APS DCOMP Student Travel Award**
APS March Meeting 2019
- 2018 **Graduate Student Research Highlight for October 2018**
Department of Chemistry, State University of New York at Buffalo
- GSEU Professional Development Award**
State University of New York at Buffalo
- 2017 **Third Place Poster Award in Graduate Category**
New York State APS Symposium

Professional Service

Editorial Board

Aug. 2020 **Condensed Matter**: Reviewer Board Member

Manuscript Reviewer

- Aug. 2021 **Physical Review B**
- July 2021 **Electronics**
- Jun. 2021 **Physical Review Letters**
Chemistry & Biodiversity
- Apr. 2021 **Physical Review Letters**

Professional Service (continued)

- Mar. 2021 ■ *Chemistry & Biodiversity*
- Mar. 2021 ■ *Crystals*
- Feb. 2021 ■ *Physical Review B*
- *Materials*
- Jan. 2021 ■ *Journal of Physical Chemistry Letters*
- Nov. 2020 ■ *Chemistry & Biodiversity*
- Sep. 2020 ■ *ChemistrySelect*
- July 2019 ■ *The Journal of Physical Chemistry*
- May 2019 ■ *Chemistry & Biodiversity*
- Jan. 2019 ■ *Scientific Reports*
- Oct. 2018 ■ *Scientific Reports*
- Sep. 2018 ■ *Chemistry & Biodiversity*
- June 2018 ■ *Physica Status Solidi B: Basic Solid State Physics*
- Feb. 2018 ■ *Computational Materials Science*

Conference Session Chair

- Mar. 2021 ■ **APS March Meeting 2021**
- Mar. 2019 ■ **APS March Meeting 2019**
- Aug. 2017 ■ **254th ACS National Meeting**

Presentations

Invited Lecture

- 2021 Dec. 16 ■ **Chicago/DOE Alliance Center (CDAC) Webinar**
“To Superconduct or Not? A Tale of Four Hydrides under Pressure”
- 2018 Nov. 27 ■ **Departmental Seminar, Laboratory for Laser Energetics, University of Rochester**
“Structure Prediction and Density Functional Theory: Searching for High-Temperature Superconductivity under High Pressure”

Contributed Presentations

- 2021 July 26 ■ **Conference on Science at Extreme Conditions (CSEC-2021)**
Talk: “The Li-F-H Ternary System at High Pressures”
- 2021 Mar. 16 ■ **APS March Meeting 2021**
Talk: “The Li-F-H Ternary System at High Pressures”
- 2020 Apr. 22 ■ **Dissertation Defense for Ph.D. in Chemistry, State University of New York at Buffalo**
Talk: “Density Functional Theory (DFT) Studies of Hydrogen Rich Materials, Methylammonium Lead Bromide Perovskite and Silicon Dioxide Under Pressure”
- 2020 Mar. 04 ■ **APS March Meeting 2020**
Talk: “Charge Transfer Induced Band Gap Closure: Trend in Rare Earth Tetrahydrides Discovered under Pressure”
- 2020 Feb. 21 ■ **The HEDPt-UB Mini-Workshop, Laboratory for Laser Energetics, University of Rochester**
Talk: “Electronic Structure and Superconductivity of Compressed Metal Tetrahydrides”

Presentations (continued)

- 2019 Mar. 04-08 **■ APS March Meeting 2019**
Talk: “Theoretical Investigation of Ternary Hydrogen-Rich Materials under Pressure”
- 2019 Feb. 18-20 **■ Stewardship Science Academic Programs (SSAP) Symposium**
Poster: “Crystal Structures and Properties of Hydrogen Rich Materials at High Pressure”
- 2018 July 14-20 **■ High Pressure Research at Gorden Research Seminar/Conference**
Poster: “Theoretical Investigation of Sodalite-Like Hydrogen Rich Materials under Pressure: Stabilization of Metallic Hydrogen Lattice”
- 2018 Feb. 21-22 **■ Stewardship Science Academic Programs (SSAP) Symposium**
Poster: “Theoretical Investigation on Phosphorus Boron Polyhydrides (PBH_n) Ternary System Under Pressure”
- 2017 Aug. 20-24 **■ 254th ACS National Meeting**
Talk: “Superconducting Phases of Phosphorus Hydride Under Pressure: Stabilization via Mobile Molecular Hydrogen”
- 2017 Apr. 21-22 **■ New York State APS Symposium**
Poster: “Superconducting Phases of Phosphorus Hydride under Pressure: Stabilization via Mobile Molecular Hydrogen”
- 2017 Apr. 12-13 **■ Stewardship Science Academic Programs (SSAP) Symposium**
Poster: “Superconducting Phases of Phosphorus Hydride Under Pressure: Stabilization via Mobile Molecular Hydrogen”
- 2016 July 16-22 **■ High Pressure Research at Gorden Research Seminar/Conference**
Poster: “Theoretical Investigation of PH_n Phases from Ambient to High Pressure”

Skills

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| Languages | ■ Professional level speaking, writing, and reading in Chinese and English. |
| Coding | ■ Python, R |
| Computational Chemistry | ■ Vienna <i>Ab Initio</i> Package (VASP), Molecular Dynamics, Quantum Espresso, Amsterdam Density Functional (ADF), LOBSTER, Phonopy, XTALOPT |
| Others | ■ Academic research, teaching, training, consultation, \LaTeX typesetting and publishing. |