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Michael Y. Toriyama

Quick Rundown

- ★ Skilled in computational materials science, particularly for energy materials
- ★ Published 11 peer-reviewed papers as first author or co-first author
- ★ Recipient of the DOE Computational Science Graduate Fellowship and Barry Goldwater Scholarship

Education

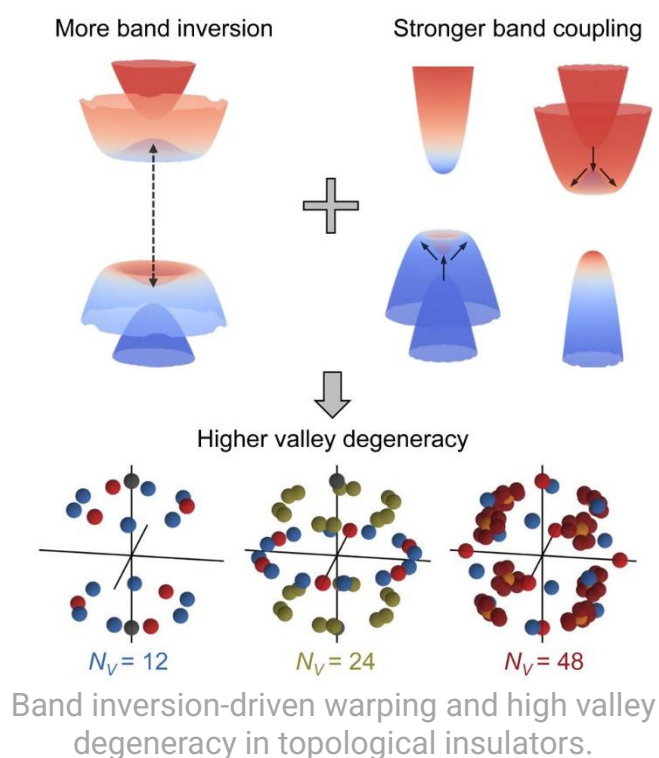
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| Northwestern University <i>Ph. D. Candidate, Materials Science and Engineering</i> | 09/2019 – Present |
| University of Illinois at Urbana-Champaign <i>Bachelor of Science, Materials Science and Engineering (High Honors)</i> <i>Bachelor of Science, Applied Mathematics (Magna Cum Laude)</i> <i>Minor, Physics</i> | 09/2015 – 05/2019 |

Research Experience

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|---|-------------------|
| Graduate Student Researcher <i>Northwestern University</i> <i>Advisors: Prof. G. Jeffrey Snyder and Prof. Prashun Gorai</i> | 09/2019 – Present |
| Students Pushing Innovation Intern <i>National Center for Supercomputing Applications</i> <i>Advisors: Prof. Elif Ertekin and Dr. Lídia Carvalho Gomes</i> | 08/2018 – 08/2019 |
| Undergraduate Researcher <i>Radiation Surface Science and Engineering Laboratory</i> <i>Advisors: Prof. Jean Paul Allain and Dr. Michael A. Lively</i> | 02/2016 – 08/2019 |
| Future Leaders of Advanced Materials Intern <i>University of California, Santa Barbara</i> <i>Advisors: Prof. Anton Van der Ven and Dr. Jonas L. Kaufman</i> | 06/2018 – 08/2018 |
| Undergraduate Intern <i>Illinois Geometry Laboratory</i> <i>Advisors: Prof. Ivan Contreras and Dr. Sarah Loeb</i> | 08/2016 – 05/2018 |
| DOE SULI Intern <i>Argonne National Laboratory</i> <i>Advisors: Dr. Maria K.Y. Chan and Dr. Fatih G. Sen</i> | 06/2017 – 08/2017 |

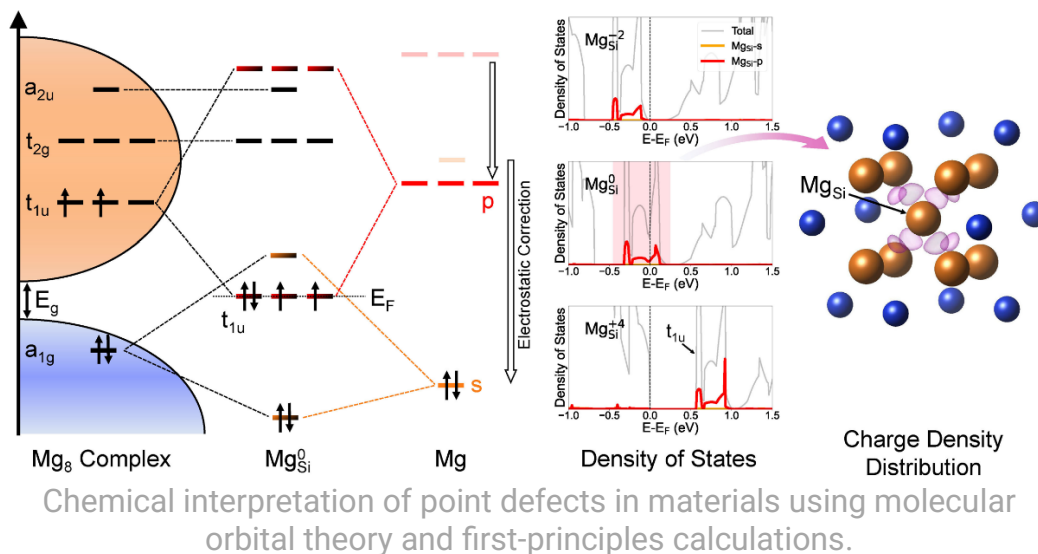
Publications

1. **M.Y. Toriyama**, A.N. Carranco, G.J. Snyder, and P. Gorai, Material Descriptors for Thermoelectric Performance of Narrow-gap Semiconductors and Semimetals, *Mater. Horiz.*, Accepted (2023).
2. **M.Y. Toriyama** and G.J. Snyder, Band Inversion-Driven Warping and High Valley Degeneracy, *Cell Rep. Phys. Sci.*, 4, 101392 (2023).



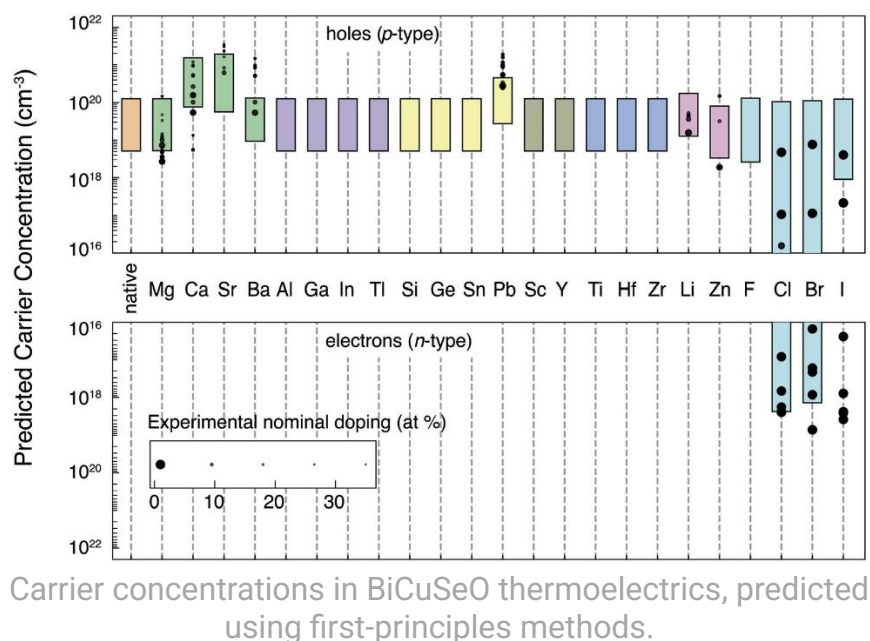
3. L.E. Borgsmiller, Q. Li, **M.Y. Toriyama**, and G.J. Snyder, New Zintl Phase $\text{Yb}_{10}\text{MgSb}_9$ with High Thermoelectric Performance, *Adv. Energy Mater.*, 2300393 (2023).
4. E. Isotta, **M.Y. Toriyama**, A.H. Adekoya, R. Shupp, G.J. Snyder, and A. Zevalkink, Effect of Sn Oxides on the Thermal Conductivity of Polycrystalline SnSe, *Mater. Today Phys.*, 31, 100967 (2023).
5. **M.Y. Toriyama**, J. Qu, L.C. Gomes, and E. Ertekin, VTAnDeM: A Python Toolkit for Simultaneously Visualizing Phase Stability, Defect Energetics, and Carrier Concentrations of Materials, *Comp. Phys. Commun.*, 287, 108691 (2023).
6. **M.Y. Toriyama**, D. Cheikh, S.K. Bux, G.J. Snyder, and P. Gorai, Y_2Te_3 : A New n-Type Thermoelectric Material, *ACS Appl. Mater. Interfaces*, 14, 43517 (2022).
7. H. Jang, **M.Y. Toriyama**, S. Abbey, B. Frimpong, J.P. Male, G.J. Snyder, Y.S. Jung, and M. Oh, Suppressing Charged Cation Antisites via Se Vapor Annealing Enables p-Type Dopability in $\text{AgBiSe}_2\text{-SnSe}$ Thermoelectrics, *Adv. Mater.*, 2204132 (2022).

8. **M.Y. Toriyama**, M.K. Brod, and G.J. Snyder, Chemical Interpretation of Charged Point Defects in Semiconductors: A Case Study of Mg_2Si , *ChemNanoMat*, 8, e202200222 (2022).



9. S. Anand, **M.Y. Toriyama**, C. Wolverton, S.M. Haile, and G.J. Snyder, A Convergent Understanding of Charged Defects, *Acc. Mater. Res.*, 3, 685 (2022).
10. **M.Y. Toriyama**, A.M. Ganose, M. Dylla, S. Anand, J. Park, M.K. Brod, J.M. Munro, K.A. Persson, A. Jain, and G.J. Snyder, How to Analyse a Density of States, *Mater. Today Electron.*, 1, 100002 (2022).
11. **M.Y. Toriyama**, M.K. Brod, L.C. Gomes, F.A. Bipasha, B.A. Assaf, E. Ertekin, and G.J. Snyder, Tuning High Valley Degeneracy in Rock-Salt IV-VI Compounds with Band Inversion, *J. Mater. Chem. A*, 10, 1588 (2022).
12. Y. Liu*, **M.Y. Toriyama***, Z. Cai, M. Zhao, F. Liu, G.J. Snyder, Finding the Order in Complexity: The Electronic Structure of 14-1-11 Zintl Compounds, *Appl. Phys. Lett.*, 119, 213902 (2021).
13. J. Qu, C.E. Porter, L.C. Gomes, J.M. Adamczyk, **M.Y. Toriyama**, B.R. Ortiz, E.S. Toberer, E. Ertekin, Controlling Thermoelectric Transport via Native Defects in the Diamond-Like Semiconductors $\text{Cu}_2\text{HgGeTe}_4$ and Hg_2GeTe_4 , *J. Mater. Chem. A*, 9, 26189 (2021).
14. M. Wood*, **M.Y. Toriyama***, S. Dugar*, J. Male, S. Anand, V. Stevanovic, and G.J. Snyder, Phase Boundary Mapping of Tin-Doped ZnSb Reveals Thermodynamic Route to High Thermoelectric Efficiency, *Adv. Energy Mater.*, 11, 2100181 (2021).
15. X. Zhang, **M.Y. Toriyama**, J.P. Male, Z. Feng, S. Guo, T. Jia, Z. Ti, G.J. Snyder, and Y. Zhang, First Principles Investigation of Intrinsic and Na Defects in XTe (X = Ca, Sr, Ba) Nanostructured PbTe, *Mater. Today Phys.*, 19, 100415 (2021).
16. N.A. Pieczulewski, M. Wood, **M.Y. Toriyama**, J.P. Male, K.J. Griffith, and G.J. Snyder, Possibility of Interstitial Na as Electron Donor in $\text{Yb}_{14}\text{MgSb}_{11}$, *MRS Comm.*, 11, 226 (2021).

17. **M.Y. Toriyama**, J. Qu, G.J. Snyder, and P. Gorai, Defect Chemistry and Doping of BiCuSeO, *J. Mater. Chem. A*, 9, 20685 (2021).



Carrier concentrations in BiCuSeO thermoelectrics, predicted using first-principles methods.

18. R. Orenstein, J.P. Male, **M.Y. Toriyama**, S. Anand, and G.J. Snyder, Using Phase Boundary Mapping to Resolve Discrepancies in the Mg₂Si-Mg₂Sn Miscibility Gap, *J. Mater. Chem. A*, 9, 7208 (2021).

19. M.K. Brod, **M.Y. Toriyama**, and G.J. Snyder, Orbital Chemistry that Leads to High Valley Degeneracy in PbTe, *Chem. Mater.*, 32, 9771-9779 (2020).

20. I.C. Contreras, **M. Toriyama**, and C. Yu, Gluing of Graph Laplacians and Their Spectra, *Linear Multilinear A*, 68, 710 (2020).

21. M.A. Lively, B. Holybee, **M. Toriyama**, S. Facsko, and J.P. Allain, Nonlinear Compositional and Morphological Evolution of Ion-Irradiated GaSb Prior to Nanostructure to Formation, *Sci. Rep.*, 10, 1 (2020).

22. A.K.M. Kanakkithodi, **M. Toriyama**, F.G. Sen, M.J. Davis, and M. Chan, Machine Learned Impurity Level Prediction for Semiconductors: the Example of Cd-Based Chalcogenides, *npj Comput. Mater.*, 6, 1 (2020).

23. **M. Toriyama**, J. Kaufman, and A. Van der Ven, Potassium Ordering and Structural Phase Stability in Layered K_xCoO₂, *ACS Appl. Energy Mater.*, 2, 2629 (2019).

24. M.A. Lively, B. Holybee, **M. Toriyama**, and J.P. Allain, Massive-Scale Molecular Dynamics of Ion-Irradiated III-V Compound Semiconductors at the Onset of Nanopatterning, *Nucl. Instrum. Meth. B*, 409, 282 (2017).



Conference Talks

1. Material Descriptors to Predict Thermoelectric Performance of Narrow-Gap Semiconductors and Semimetals, International Conference on Thermoelectrics, Seattle, WA (June 23, 2023).
2. Band Inversion-Driven Warping for Achieving High Valley Degeneracy, International Conference on Thermoelectrics, Seattle, WA (June 22, 2023).
3. Band Inversion-Driven High Valley Degeneracy, MRS Fall Meeting, Boston, MA (December 1, 2022).
4. Material Descriptors to Search for Low-Temperature Thermoelectric Materials, MRS Fall Meeting, Boston, MA (November 28, 2022).
5. Band Inversion-Driven High Valley Degeneracy, Virtual Conference on Thermoelectrics (July 20, 2022).
6. Chemically Tuning Non-Parabolic Electronic Structures in Rock-Salt IV-VI Compounds, MRS Fall Meeting, Boston, MA (November 29, 2021).
7. Defect Chemistry and Doping of BiCuSeO, Virtual Conference on Thermoelectrics (July 20, 2021).
8. Chemistry of Point Defects: Case Study of Mg_{Si} in Mg_2Si , Virtual Conference on Thermoelectrics (July 23, 2020).
9. Graph Theory-Based Gluing Formulae for Electronic Structure Calculations, SRC TECHCON 2018, Austin, TX (September 16-19, 2018).
10. Computational Studies of Ion Irradiation Effects on GaSb Surfaces, Tau Beta Pi Research Symposium, University of Illinois at Urbana-Champaign (April 17, 2018).
11. Gluing Graphs and Electronic Structures of Matter, Undergraduate Mathematics Symposium, University of Illinois at Chicago (November 18, 2017).



Professional Experience

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| Conference Organizer <i>Virtual Conference on Thermoelectrics</i> | 2021, 2022 |
| Teaching Assistant, Northwestern University <i>MAT_SCI 351-2 (Intro Physics of Materials)</i> | Winter 2022, 2023 |
| Teaching Assistant, UIUC <i>MATH 286 (Differential Equations)</i> | Fall 2018 |

Mentoring

Master's Students

- **Junjie Wang** Present
Northwestern University
Project: Enhancing Thermoelectric Performance with Magnetic Fields
- **Jordan Miller** 2021–2022
Northwestern University
Project: Defect Chemistry of Distorted Defects in MgO

Undergraduate Students

- **Louis Wong** 2023
Northwestern University
Project: Defect Chemistry of SrTiO₃ and Ceria Using MO Theory
- **Andrew Borland** 2022
Northwestern University
Project: Computational Discovery of Oxychalcogenides Using ML
- **Adam Carranco** 2021–2022
MURF (Colorado School of Mines)
Project: Discovery of New Low-Temperature Thermoelectric Materials
- **Alessandro Pereyra** Summer 2020
MRSEC REU
Project: Analysis of Thermoelectrics Data
- **Johnny Tran** Summer 2020
MRSEC REU
Project: Analysis of Thermoelectrics Data

High School Students

- **Huzaifa Saif** Summer 2023
Troy Tech Senior internship (Troy High School)
Project: Web Development for Thermoelectric Transport Analysis
- **Estefanny Ruiz** Summer 2019
High School Summer Research Program (Urbana High School)
Project: Phase Stability Analysis for Thermoelectrics



Honors and Awards

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| DOE Computational Science Graduate Fellowship | 2019–2023 |
| Hilliard Symposium (2nd Place) | 2023 |
| Dean's List | 2015–2019 |
| TECHCON Undergraduate Poster Award (3rd Place) | 2018 |
| Barry Goldwater Scholarship | 2018 |
| Cullen W. Parmelee Scholarship | 2016, 2018 |
| Wert Scholarship | 2017 |
| Illinois Geometry Laboratory Research Award (1st Place) | 2017 |
| Alfred W. Allen Award | 2016 |
| Engineering Open House Best Freshman Exhibit (2nd Place) | 2016 |