

Materials@AState

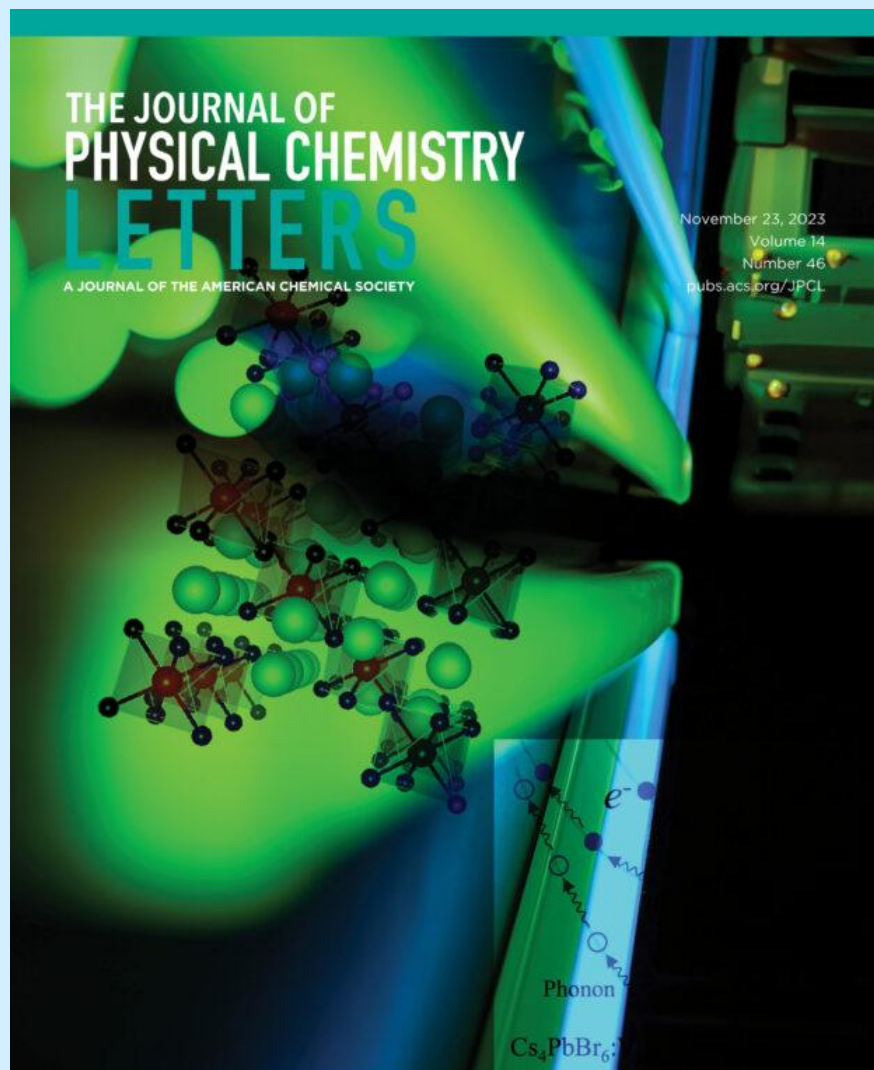
Biswas Group's Research Page

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Recent News and Publications

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Comet Tsuchinshan-ATLAS as viewed from Northeast Arkansas (mid-October 2024)

Credit: Justin Crossno, Arkansas State University.



Northern Lights as viewed from Northeast Arkansas (mid-November 2025)

Credit: Henry Mahan, Arkansas State University

Recent Publications

[The nature of defect tolerance in \(some\) halide perovskites](#)

[The halogen vacancy, Tl-activator, and Tl-bound excitons in CsI:Tl scintillator](#)

[Presentation on \$\text{Cs}_2\text{HfCl}_6\$](#)

[Case of the Bromine Vacancy in \$\text{Cs}_4\text{PbBr}_6\$ \(Journal of Physical Chemistry Letters\)](#)

[Revisiting the origin of green emission in \$\text{Cs}_4\text{PbBr}_6\$ \(Materials Advances\)](#)

[Metal Halide Semiconductors beyond Lead-Based Perovskites for Promising Optoelectronic Applications \(Journal of Physical Chemistry Letters\)](#)

[Phase transition pathway of hybrid halide perovskites under compression: Insights from first-principles calculations \(Phys. Rev. Materials\)](#)

[New Polymorphs of 2D Indium Selenide with Enhanced Electronic Properties \(Advanced Functional Materials\)](#)

Research

We are interested in first-principles based or empirical and semi-empirical methods to study, characterize, and optimize materials for optoelectronic applications. Excerpts from some of our recent works are shown below as a brief overview.

Support

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Publications

1. K. Biswas, "The nature of defect tolerance in (some) halide perovskites", [*APL Electronic Devices* **1**, 030901 \(2025\)](#).
2. B. Kang and K. Biswas, "The halogen vacancy, TI-activator, and TI-bound excitons in CsI:TI scintillator", [*J. Appl. Phys.* **138**, 135105 \(2025\)](#).
3. B. Kang and K. Biswas, "Case of the Bromine Vacancy in Cs_4PbBr_6 ", [*J. Phys. Chem. Lett.* **14**, 10378 \(2023\)](#).
4. K. Biswas, "Revisiting the origin of green emission in Cs_4PbBr_6 ", [*Mater. Adv.* **3**, 6791-6798 \(2022\)](#).
5. X. Wang et al., "Metal Halide Semiconductors beyond Lead-Based Perovskites for Promising Optoelectronic Applications", [*J. Phys. Chem. Lett.* **12**, 10532 \(2021\)](#).
6. D. Yang et al., "Phase transition pathway of hybrid halide perovskites under compression: Insights from first-principles calculations", [*Phys. Rev. Mater.* **5**, 054603 \(2021\)](#).
7. Y. Sun et al., "New Polymorphs of 2D Indium Selenide with Enhanced Electronic Properties", [*Advanced Functional Materials*, 2001920 \(2020\)](#).
8. Q. Xu et al., "Impact of organic molecule rotation on the optoelectronic properties of hybrid halide perovskites", [*Phys. Rev. Mater.* **3**, 125401 \(2019\)](#).
9. X. Wang, Z. Liu, X-G Zhao, J. Lv, K. Biswas*, and, L. Zhang*, "Computational Design of Mixed-Valence Tin Sulfides as Solar Absorbers", [*ACS Appl. Mater. Interfaces* **11**, 24867 \(2019\)](#).
10. B. Kang and K. Biswas, "Exploring Polaronic, Excitonic Structures and Luminescence in $\text{Cs}_4\text{PbBr}_6/\text{CsPbBr}_3$ ", [*J. Phys. Chem. Lett.* **9**, 830 \(2018\)](#).
11. Z. Ran, X. Wang, Y. Li, D. Yang, X-G. Zhao, K. Biswas, D. J. Singh, and L. Zhang, "Bismuth and antimony-based oxyhalides and chalcogenides as potential optoelectronic materials", [*npj Computational Materials* **4**, Article number: 14 \(2018\)](#).
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16. Q. Feng, R. Noubissi, K. Biswas, and H. Koizumi, "The role of hydroxyl groups in interchain interactions in cellulose I_α and I_β " *Int. J. Quantum Chemistry* **117**, e25357 (2017).
17. Q. Feng and K. Biswas, "Ramifications of codoping $SrI_2:Eu$ with isovalent and aliovalent impurities" *J. Appl. Phys.* **120**, 213104 (2016).
18. By. Kang, C. M. Fang, and K. Biswas, "A first-principles based study of ns^2 containing ternary iodides and their possibility of scintillation" *J. Phys. D: Appl. Phys.* **49**, 395103 (2016).
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Book Chapter

Invited Presentations

1. K. Biswas (2023) “Carrier Self-trapping and Luminescence in Cesium Hafnium Chloride”, Virtual Talk, Department of Physics Colloquium, Alabama A&M University.
2. K. Biswas (2019) “Hybrid and All-Inorganic Perovskite Halides”, Condensed Matter Seminar, Texas A&M University, September, 2019.
3. K. Biswas (2018) “Structural and Property Trends Among Complex Halides”, Seminar, University of Memphis, October, 2018.
4. K. Biswas (2018) “A Brief Perspective on Halides as Optoelectronic Materials”, Seminar, Jilin University – China, June, 2018.
5. K. Biswas (2014) “Search for improved-performance scintillator candidates among the electronic structures of mixed halides”, SPIE Optics+Photonics, San Diego, CA, August, 2014.
6. K. Biswas (2014) “Impurities in TlBr”, TlBr Workshop & Review Meeting, University of Michigan, Ann Arbor, MI, June, 2014.
7. K. Biswas (2014) “Scintillation Mechanisms in Gamma Detectors – Electronic Structure Theory”, Department of Energy-National Nuclear Security Administration, Washington, DC, April, 2014.
8. K. Biswas (2013) “Density functional models of semiconductors”, TlBr Workshop & Review Meeting, Harvard University, Cambridge, MA, September 19, 2013.
9. K. Biswas (2013) “DFT based study of materials for radiation detector application”, 6th DNDONSF Annual Academic Research Initiative (ARI) Grantees Program Review, Leesburg, VA, July, 2013.
10. K. Biswas (2013) “DFT Studies of Semiconductor and Scintillator Detection Materials”, 2013 March meeting of the American Physical Society, Baltimore, MD, Mar, 2013.
11. K. Biswas (2012) “Materials for application in photovoltaics and optoelectronics”, Applied Materials Science Division, Saha Institute of Nuclear Physics, Calcutta, India, May, 2012.
12. K. Biswas (2012) “Materials for application in photovoltaics and optoelectronics”, Graduate Seminar Series, Materials Science and Engineering Department, University of Tennessee, Knoxville, February, 2012.