

Department of Chemistry & Physics

- [Materials@AState](#)
 - [Recent News and Publications](#)
 - [Research](#)
 - [Publications](#)

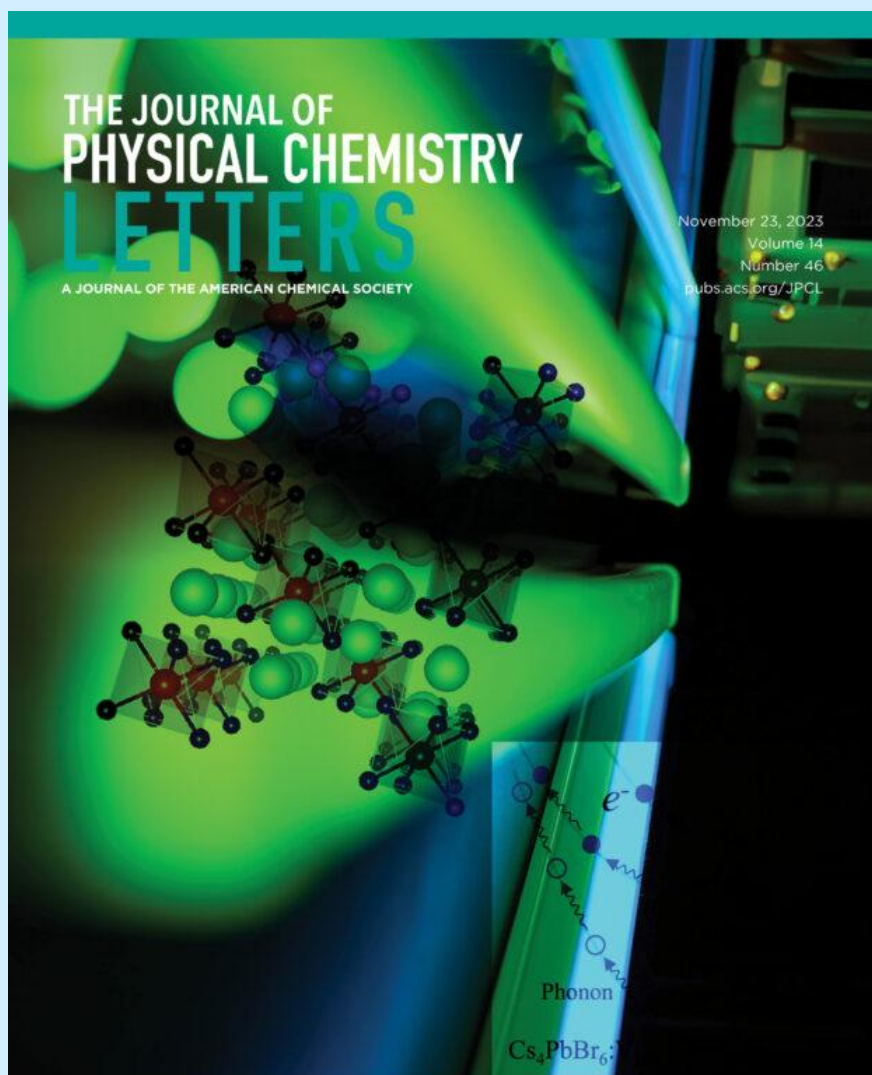
Materials@AState

Biswas Group's Research Page

Recent News and Publications

JPCL Cover Image

Nov. 23, 2023; Volume 14, Issue 46





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 \(Advanced Functional Materials\)](#)

Materials@AState

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

Our research is supported by the National Science Foundation (NSF), Department of Homeland Security (DHS), and Arkansas State University.

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, Tl-activator, and Tl-bound excitons in CsI:Tl 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 \(2018\)](#).
12. Y. Sun, S. Luo, X-G Zhao, K. Biswas, S-L Li, and L. Zhang, "InSe: a two-dimensional material with strong interlayer coupling", [*Nanoscale* DOI: 10.1039/C7NR09486H \(2018\)](#).
13. B. Kang, Q. Feng, and K. Biswas, "Comparative study of perovskite-type scintillator materials CsCaI_3 and KCaI_3 via first-principles calculations", [*J. Phys. D: Appl. Phys.* **51**, 065303 \(2018\)](#).
14. B. Kang and K. Biswas, "Shallow trapping vs. deep polarons in a hybrid lead halide perovskite, $\text{CH}_3\text{NH}_3\text{PbI}_3$ ", [*Physical Chemistry Chemical Physics* **19**, 27184 \(2017\)](#).
15. B. Kang and K. Biswas, "Preferential CH_3NH_3^+ Alignment and Octahedral Tilting Affect Charge Localization in Cubic Phase $\text{CH}_3\text{NH}_3\text{PbI}_3$ ", [*Journal of Physical Chemistry C* **121**,](#)

[8319 \(2017\)](#).

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 \(2016\)](#).
19. By. Kang and K. Biswas, "Carrier Self-trapping and Luminescence in Intrinsically Activated Scintillator: Cesium Hafnium Chloride (Cs_2HfCl_6)" [Journal of Physical Chemistry C **120**, 12187 \(2016\)](#).
20. C-M Fang and K. Biswas, "Quaternary Iodides $A(BaSr)I_5:Eu^{2+}$ ($A = K, Cs$) as Scintillators for Radiation Detection" [Journal of Physical Chemistry C **120**, 1225 \(2016\)](#).
21. Kang et al., "Emerging New Pseudobinary and Ternary Halides as Scintillators for Radiation Detection" [IEEE Transactions on Nuclear Science \(2016\)](#).
22. C-M Fang and K. Biswas, "Preferential Eu Site Occupation and Its Consequences in the Ternary Luminescent Halides $AB_2I_5:Eu^{2+}$ ($A=Li-Cs$; $B=Sr, Ba$)" [Physical Review Applied **4**, 014012 \(2015\)](#).
23. R. Adhikari, Q. Li, R. Williams, A. Burger, and K. Biswas, "DX-like centers in $NaI:Tl$ upon aliovalent codoping" [Journal of Applied Physics **116**, 223703 \(2014\)](#).
24. Q. Li, R. T. Williams, A. Burger, R. Adhikari, and K. Biswas, "Search for improved-performance scintillator candidates among the electronic structures of mixed halides", [Proceedings of SPIE **9213**, 92130M \(2014\)](#).
25. M.-H. Du and K. Biswas, "Electronic structure engineering of elpasolites: Case of Cs_2AgYCl_6 " [Journal of Luminescence **143**, 710 \(2013\)](#).
26. K. Biswas, M.-H. Du, and D. J. Singh "Electronic structure and defect properties of Tl_6SeI_4 : Density functional calculations" [Physical Review B **86**, 144108 \(2012\)](#).
27. K. Biswas, M.-H. Du, J. T-Thienprasert, S. Limpijumnong, and D. J. Singh, Comment on "Uncovering the complex behavior of hydrogen in Cu_2O " [Physical Review Letters **108**, 219703 \(2012\)](#).
28. K. Biswas and M.-H. Du, "Energy transport and scintillation of Cerium doped elpasolite Cs_2LiYCl_6 : hybrid density functional calculations" [Physical Review B **86**, 014102 \(2012\)](#).
29. K. Biswas and M.-H. Du, "What Causes of high resistivity in $CdTe$ " [New Journal of Physics **14**, 063020 \(2012\)](#).
30. M.-H. Du and K. Biswas, "Anionic and hidden hydrogen in ZnO ", [Physical Review Letters **106**, 115502 \(2011\)](#).

31. K. Biswas and M.-H. Du, "AX centers in II-VI semiconductors: Hybrid Functional Calculations", [*Applied Physics Letters* **98**, 181913 \(2011\)](#).
32. M.-H. Du, K. Biswas, and D. J. Singh, "Electronic structure, energy transport, and optical properties of halide scintillators", [*Proceedings of SPIE* **8507**, 850705 \(2012\)](#).
33. M.-H. Du, K. Biswas, and D. J. Singh, "Resistivity, carrier trapping, and polarization phenomenon in semiconductor radiation detection materials", [*Proceedings of SPIE***8507**, 85070M \(2012\)](#).
34. G. Trimarchi, H. Peng, J. Im, A. J. Freeman, V. Cloet, A. Raw, K. R. Poeppelmeier, K. Biswas, S. Lany, and A. Zunger, "Using design principles to systematically plan the synthesis of hole-conducting transparent oxides: Cu_3VO_4 and Ag_3VO_4 as a case study", [*Physical Review B* **84**, 165116 \(2011\)](#).
35. K. Biswas and M.-H. Du, "First principles study of native defects in InI", [*Journal of Applied Physics* **109**, 113518 \(2011\)](#).
36. K. Biswas, S. Lany, and A. Zunger, "The electronic consequences of multivalent elements in inorganic solar absorbers: Multivalency of Sn in $\text{Cu}_2\text{ZnSnS}_4$ ", [*Applied Physics Letters* **96**, 201902 \(2010\)](#).
37. M. Beekman, E. N. Nenghabi, K. Biswas, C. W. Myles, M. Baitinger, Y. Grin, and G. S. Nolas, "Framework Contraction in Na-Stuffed Si(cF 136)", [*Inorganic Chemistry* **49**, 5338 \(2010\)](#).
38. K. Biswas and S. Lany, "Energetics of quaternary III-V alloys described by incorporation and clustering of impurities", [*Physical Review B* **80**, 115206 \(2009\)](#).
39. K. Biswas, A. Franceschetti, and S. Lany, "Generalized valence-force-field model of (Ga,In)(N,P) ternary alloys", [*Physical Review B* **78**, 085212 \(2008\)](#).
40. K. Biswas, C. W. Myles, M. Sanati, and G. S. Nolas "Thermal properties of guest-free Si_{136} and Ge_{136} clathrates: A first-principles study", [*Journal of Applied Physics* **104**, 033535 \(2008\)](#).
41. K. Biswas and C. W. Myles, "Electronic and vibrational properties of framework-substituted type-II Si clathrates", [*Physical Review B* **75**, 245205 \(2007\)](#).
42. K. Biswas and C. W. Myles, "Density-functional investigation of $\text{Na}_{16}\text{A}_8\text{Ge}_{136}$ (A=Rb,Cs)clathrates", [*Journal of Physics: Condensed Matter* **19**, 466206 \(2007\)](#).
43. K. Biswas and C. W. Myles, "Electronic properties of the $\text{Na}_{16}\text{Rb}_8\text{Si}_{136}$ and $\text{K}_{16}\text{Rb}_8\text{Si}_{136}$ clathrates", [*Physical Review B* **74**, 115113 \(2006\)](#).
44. C. W. Myles, K. Biswas, and E. Nenghabi, "Rattling guest impurities in Si and Ge clathrate semiconductors", [*Physica B* **401**, 695 \(2007\)](#).
45. K. Biswas, S. Gangopadhyay, H. C. Kim, and R. D. Miller, "Nanoporous organosilicate films as antireflection coatings", [*Thin Solid Films* **514**, 350 \(2006\)](#).
46. S. Gangopadhyay, J. A. Lubguban, B. Lahlouh, G. Sivaraman, K. Biswas, T. Rajagopalan, N. Biswas, H.-C. Kim, W. Volksen, R. D. Miller, "Supercritical CO₂ Treatments for Semiconductor Applications", [*MRS Proceedings* **812**, F4.6 \(2004\)](#).

Book Chapter

[Perovskites – Revisiting the Venerable \$ABX_3\$ Family with Organic Flexibility and New Applications](#), in *Optical Properties of Materials and Their Applications*, 2nd Ed. (Wiley)

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.