

**Curriculum Vitae**  
**Koushik Biswas, Ph.D.**  
Contact Email: [kbiswas@astate.edu](mailto:kbiswas@astate.edu)  
Website: <https://materials.astate.edu/>

**CURRENT POSITION** Associate Professor of Physics, Arkansas State University

**EDUCATION**

2007 PhD (Physics), Texas Tech University, Lubbock, TX  
1999 MSc. (Physics) Jadavpur University, Calcutta, India  
1997 BSc. (Physics) Kharagpur College, Kharagpur, India

**POSTDOCTORAL TRAINING**

7/2010 – 8/2012 Postdoctoral Researcher, Advanced Materials Group, Oak Ridge National Laboratory (ORNL)  
8/2007 – 7/2010 Postdoctoral Researcher, Solid State Theory Group, National Renewable Energy Laboratory (NREL)

**APPOINTMENT**

7/2017 – present Associate Professor of Physics (tenured), Arkansas State University, Jonesboro  
8/2012 – 6/2017 Tenure Track Assistant Professor of Physics, Arkansas State University, Jonesboro

**RESEARCH INTERESTS**

We focus on first-principles based computational investigation and development of electronic materials. They include bulk, low-dimensional materials and heterostructures that are important in photovoltaics, photocatalysis, light emitting devices, and radiation detection. We strive to maintain collaborative efforts with experimental researchers working in similar fields.

**PEER-REVIEWED PUBLICATIONS**

1. **K. Biswas**, “Revisiting the origin of green emission in Cs<sub>4</sub>PbBr<sub>6</sub>”, *Mater. Adv.* **3**, 6791-6798 (2022). <https://doi.org/10.1039/D2MA00544A>
2. D. Yang, Y. Fu, Y. Sun, Y. Li, K. Wang, Z. Xiao, **K. Biswas**, and L. Zhang, “Phase transition pathway of hybrid halide perovskites under compression: Insights from first-principles calculations”, *Phys. Rev. Materials* **5**, 054603 (2021). <https://doi.org/10.1103/PhysRevMaterials.5.054603>
3. X. Wang, T. Li, B. Xing, M. Faizan, **K. Biswas**, and L. Zhang, “Metal Halide Semiconductors beyond Lead-Based Perovskites for Promising Optoelectronic Applications”, *J. Phys. Chem. Lett.* **12**, 10532 (2021). <https://doi.org/10.1021/acs.jpcclett.1c02877>
4. Y. Sun, Y. Li, T. Li, **K. Biswas**, A. Patanè, and L. Zhang, “New Polymorphs of 2D Indium Selenide with Enhanced Electronic Properties”, *Advanced Functional Materials* **30**, 2001920 (2020). <https://doi.org/10.1002/adfm.202001920>
5. Q. Xu, A. Stroppa, J. Lv, X. Zhao, D. Yang, **K. Biswas**, and L. Zhang, “Impact of organic molecule rotation on the optoelectronic properties of hybrid halide perovskites”, *Phys. Rev. Materials* **3**, 125401 (2019). <https://doi.org/10.1103/PhysRevMaterials.3.125401>
6. 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 Applied Materials & Interfaces* **11**, 24867 (2019). <https://doi.org/10.1021/acsami.9b01223>
7. B. Kang and **K. Biswas**, “Exploring Polaronic, Excitonic Structures and Luminescence in Cs<sub>4</sub>PbBr<sub>6</sub>/CsPbBr<sub>3</sub>”, *J. Phys. Chem. Lett.* **9**, 830 (2018). <https://dx.doi.org/10.1021/acs.jpcclett.7b03333>
8. 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**, 14 (2018). <https://dx.doi.org/10.1038/s41524-018-0071-1>
9. 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* **10**, 7991 (2018). <https://dx.doi.org/10.1039/C7NR09486H>
10. B. Kang, Q. Feng, and **K. Biswas**, “Comparative study of perovskite-type scintillator materials CsCaI<sub>3</sub> and KCaI<sub>3</sub> via first-principles calculations”, *J. Phys. D: Appl. Phys.* **51**, 065303 (2018). <https://dx.doi.org/10.1088/1361-6463/aaa17a>
11. B. Kang and **K. Biswas**, “Shallow trapping vs. deep polarons in a hybrid lead halide perovskite, CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub>”, *Physical Chemistry Chemical Physics* **19**, 27184 (2017). <http://dx.doi.org/10.1039/C7CP04417H>
12. B. Kang and **K. Biswas**, “Preferential CH<sub>3</sub>NH<sub>3</sub><sup>+</sup> Alignment and Octahedral Tilting Affect Charge Localization in Cubic Phase CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub>”, *J. Phys. Chem. C* **121**, 8319 (2017). <http://dx.doi.org/10.1021/acs.jpcc.7b01184>
13. Q. Feng, R. Noumbissi, **K. Biswas**, and H. Koizumi, “The Role of Hydroxyl Groups in Inter-Chain Interactions in Cellulose I<sub>α</sub> and I<sub>β</sub>”, *Int. J. Quantum Chem.* **117**, e25357 (2017). <https://doi.org/10.1002/qua.25357>
14. B. Kang, Q. Feng, C. Summers, C. M. Fang, R. Adhikari, and **K. Biswas**, “Emerging New Pseudobinary and Ternary Halides as Scintillators for Radiation Detection” *IEEE Transactions on Nuclear Science* **64**, 1817 (2017). <https://doi.org/10.1109/TNS.2016.2632064>

15. Q. Feng and **K. Biswas**, “Ramifications of codoping SrI<sub>2</sub>:Eu with isovalent and aliovalent impurities”, *Journal of Applied Physics* **120**, 213104 (2016). <http://dx.doi.org/10.1063/1.4971180>
16. B. Kang, C. M. Fang, and **K. Biswas**, “A first-principles based study of ns<sup>2</sup> containing ternary iodides and their possibility of scintillation”, *J. Phys. D: Appl. Phys.* **49**, 395103 (2016). <http://dx.doi.org/10.1088/0022-3727/49/39/395103>
17. B. Kang and **K. Biswas**, “Carrier Self-trapping and Luminescence in Intrinsically Activated Scintillator: Cesium Hafnium Chloride (Cs<sub>2</sub>HfCl<sub>6</sub>)” *J. Phys. Chem. C* **120**, 12187 (2016). <http://dx.doi.org/10.1021/acs.jpcc.6b02496>
18. C. M. Fang and **K. Biswas**, “Quaternary iodides A(Ba,Sr)I<sub>5</sub>:Eu<sup>2+</sup> (A=K, Cs) as scintillators for radiation detection” *J. Phys. Chem. C* **120**, 1225 (2016). <http://dx.doi.org/10.1021/acs.jpcc.5b10690>
19. C. M. Fang and **K. Biswas**, “Preferential Eu site occupation and its consequences in the ternary luminescent halides AB<sub>2</sub>I<sub>5</sub>:Eu<sup>2+</sup> (A=Li-Cs; B=Sr,Ba)” *Phys. Rev. Appl.* **4**, 014012 (2015). <https://doi.org/10.1103/PhysRevApplied.4.014012>
20. 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). <http://dx.doi.org/10.1063/1.4903766>
21. M.-H. Du and **K. Biswas**, “Electronic structure engineering of elpasolites: Case of Cs<sub>2</sub>AgYCl<sub>6</sub>”, *Journal of Luminescence* **143**, 710 (2013). <http://dx.doi.org/10.1016/j.jlumin.2013.05.033>
22. **K. Biswas**, M.-H. Du, and D. J. Singh “Electronic structure and defect properties of Tl<sub>6</sub>SeI<sub>4</sub>: Density functional calculations” *Physical Review B* **86**, 144108 (2012). <http://dx.doi.org/10.1103/PhysRevB.86.144108>
23. **K. Biswas** and M.-H. Du, “Energy transport and scintillation of Cerium doped elpasolite Cs<sub>2</sub>LiYCl<sub>6</sub>: hybrid density functional calculations” *Physical Review B* **86**, 014102 (2012). <http://dx.doi.org/10.1103/PhysRevB.86.014102>
24. **K. Biswas** and M.-H. Du, “Causes of high resistivity in CdTe” *New Journal of Physics* **14**, 063020 (2012). <http://dx.doi.org/10.1088/1367-2630/14/6/063020>
25. **K. Biswas**, M.-H. Du, J. T-Thienprasert, S. Limpijumnong, and D. J. Singh, Comment on “Uncovering the complex behavior of hydrogen in Cu<sub>2</sub>O” *Physical Review Letters* **108**, 219703 (2012). <http://dx.doi.org/10.1103/PhysRevLett.108.219703>
26. 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<sub>3</sub>VO<sub>4</sub> and Ag<sub>3</sub>VO<sub>4</sub> as a case study”, *Physical Review B* **84**, 165116 (2011). <http://dx.doi.org/10.1103/PhysRevB.84.165116>
27. M.-H. Du and **K. Biswas**, “Anionic and hidden hydrogen in ZnO”, *Physical Review Letters* **106**, 115502 (2011). <http://dx.doi.org/10.1103/PhysRevLett.106.115502>
28. **K. Biswas** and M.-H. Du, “AX centers in II-VI semiconductors: Hybrid Functional Calculations”, *Applied Physics Letters* **98**, 181913 (2011). <http://dx.doi.org/10.1063/1.3583661>
29. **K. Biswas** and M.-H. Du, “First principles study of native defects in InI”, *Journal of Applied Physics* **109**, 113518 (2011). <http://dx.doi.org/10.1063/1.3592231>
30. **K. Biswas**, S. Lany, and A. Zunger, “The electronic consequences of multivalent elements in inorganic solar absorbers: Multivalency of Sn in Cu<sub>2</sub>ZnSnS<sub>4</sub>”, *Applied Physics Letters* **96**, 201902 (2010). <http://dx.doi.org/10.1063/1.3427433>

31. 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). <http://dx.doi.org/10.1021/ic1005049>
32. **K. Biswas** and S. Lany, “Energetics of quaternary III-V alloys described by incorporation and clustering of impurities”, *Physical Review B* **80**, 115206 (2009). <http://dx.doi.org/10.1103/PhysRevB.80.115206>
33. **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). <http://dx.doi.org/10.1103/PhysRevB.78.085212>
34. **K. Biswas**, C. W. Myles, M. Sanati, and G. S. Nolas “Thermal properties of guest-free Si<sub>136</sub> and Ge<sub>136</sub> clathrates: A first-principles study”, *Journal of Applied Physics* **104**, 033535 (2008). <http://dx.doi.org/10.1063/1.2960580>
35. **K. Biswas** and C. W. Myles, “Electronic and vibrational properties of framework-substituted type-II Si clathrates”, *Physical Review B* **75**, 245205 (2007). <http://dx.doi.org/10.1103/PhysRevB.75.245205>
36. **K. Biswas** and C. W. Myles, “Density-functional investigation of Na<sub>16</sub>A<sub>8</sub>Ge<sub>136</sub>(A=Rb,Cs)clathrates”, *Journal of Physics: Condensed Matter* **19**, 466206 (2007). <http://dx.doi.org/10.1088/0953-8984/19/46/466206>
37. C. W. Myles, **K. Biswas**, and E. Nenghabi, “Rattling guest impurities in Si and Ge clathrate semiconductors”, *Physica B* **401**, 695 (2007). <http://dx.doi.org/10.1016/j.physb.2007.09.054>
38. **K. Biswas**, S. Gangopadhyay, H. C. Kim, and R. D. Miller, “Nanoporous organosilicate films as antireflection coatings”, *Thin Solid Films* **514**, 350 (2006). <http://dx.doi.org/10.1016/j.tsf.2006.02.087>
39. **K. Biswas** and C. W. Myles, “Electronic properties of the Na<sub>16</sub>Rb<sub>8</sub>Si<sub>136</sub> and K<sub>16</sub>Rb<sub>8</sub>Si<sub>136</sub>clathrates”, *Physical Review B* **74**, 115113 (2006). <http://dx.doi.org/10.1103/PhysRevB.74.115113>

### PEER-REVIEWED PROCEEDINGS

1. 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”, *Invited Paper, Proceedings of SPIE* **9213**, 92130M (2014). <http://dx.doi.org/10.1117/12.2063583>
2. 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). <http://dx.doi.org/10.1117/12.929131>
3. 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). <http://dx.doi.org/10.1117/12.930072>
4. S. Gangopadhyay, J. A. Lubguban, B. Lahlouh, G. Sivaraman, **K. Biswas**, T. Rajagopalan, N. Biswas, H.-C. Kim, W. Volksen, and R. D. Miller, “Supercritical CO<sub>2</sub> Treatments for Semiconductor Applications”, *MRS Proceedings* **812**, F4.6 (2004). <http://dx.doi.org/10.1557/PROC-812-F4.6>

### BOOK CHAPTER

“Perovskites – Revisiting the venerable ABX<sub>3</sub> family with organic flexibility and new applications”, J. Xu, David L. Carroll, **K. Biswas**, F. Moretti, S. Gridin, and R. T. Williams, book chapter in *Optical Properties of Materials and Their Applications*, 2<sup>nd</sup> Ed (Wiley, 2020). <http://doi.org/10.1002/9781119506003.ch18>

## INVITED PRESENTATIONS

1. **K. Biswas** (2019) “Hybrid and All-Inorganic Perovskite Halides: A First-Principles Perspective”, Condensed Matter Seminar, Department of Physics & Astronomy, Texas A&M University, College Station, TX.
2. **K. Biswas** (2018) “Structural and property trends among low-dimensional halide perovskites”, Seminar, Department of Physics and Materials Science, University of Memphis, TN.
3. **K. Biswas** (2018) “A brief perspective on halides as optoelectronic materials”, Seminar, College of Materials Science & Engineering, Jilin University, China.
4. **K. Biswas** (2014) “Search for improved-performance scintillator candidates among the electronic structures of mixed halides”, SPIE Optical Engineering + Applications Conference, San Diego, CA.
5. **K. Biswas** (2014) “Impurities in TlBr”, TlBr Workshop & Review Meeting (Domestic Nuclear Detection Office), University of Michigan, Ann Arbor, MI.
6. **K. Biswas** (2014) “Scintillation Mechanisms in Gamma Detectors – Electronic Structure Theory”, Department of Energy-National Nuclear Security Administration Workshop, Washington, DC.
7. **K. Biswas** (2013) “DFT Studies of Semiconductor and Scintillator Detection Materials”, March Meeting of the American Physical Society, Baltimore, MD.
8. **K. Biswas** (2013) “Density functional models of semiconductors”, TlBr Workshop & Review Meeting (Domestic Nuclear Detection Office), Harvard University, Cambridge, MA.
9. **K. Biswas** (2013) “DFT based study of materials for radiation detector application”, 6<sup>th</sup> Domestic Nuclear Detection Office-NSF Annual Academic Research Initiative (ARI) Grantees Program Review Meeting, Leesburg, VA.
10. **K. Biswas** (2012) “Materials for application in photovoltaics and optoelectronics”, Applied Materials Science Division, Saha Institute of Nuclear Physics, Calcutta, India.
11. **K. Biswas** (2012) “Materials for application in photovoltaics and optoelectronics”, Graduate Seminar Series, Materials Science and Engineering Department, University of Tennessee-Knoxville, TN.

## RECENT PRESENTATIONS & ABSTRACTS

1. Y. Sun, S-L. Li, **K. Biswas**, and L. Zhang (2019) “Computational Design of New Polymorphs of Two-dimensional Semiconductor InSe With Enhanced Interlayer Interaction”, American Physical Society March Meeting, Boston, MA.
2. **K. Biswas** and B. Kang (2018) “A Brief Perspective on Perovskite-type Halides as Highly Luminescent Materials”, IEEE Nuclear Science Symposium and Medical Imaging Conference, Sydney, Australia.
3. B. Kang and **K. Biswas** (2018) “Shallow vs. Deep Charge Localization in Hybrid Lead Halide Perovskites”, American Physical Society March Meeting, Los Angeles, CA.
4. **K. Biswas**, Q. Feng, and B. Kang (2018) “Perovskite-type Metal Halides as Luminescent Materials”, American Physical Society March Meeting, Los Angeles, CA.

5. **K. Biswas** (2018) “Physics-Driven Scintillator Design”, Domestic Nuclear Detection Office Annual Review Conference, University of Tennessee, Knoxville, TN.
6. Q. Feng, B. Kang, J. Mize, and **K. Biswas** (2017) “First-principles Study of Complex Halide Scintillators for Radiation Detection”, American Physical Society March Meeting, New Orleans, LA.
7. J. Mize, Q. Feng, B. Kang, **K. Biswas** (2017) “Investigating the Defect and Dopant Properties of CsCaI<sub>3</sub>:Eu<sup>2+</sup> for Scintillator Applications: A First-principles Study”, National Conference on Undergraduate Research, Memphis, TN.
8. J. Williams, B. Kang, and **K. Biswas** (2017) “Study of Cs<sub>2</sub>XCl<sub>6</sub> (X = Hf, Ge, Pb, Sn, Zr) Compounds”, Domestic Nuclear Detection Office Annual Review Conference, Wake Forest University, Winston-Salem, NC.
9. **K. Biswas** (2017) “Realizing High Performance Inorganic Scintillators at Low Cost”, Domestic Nuclear Detection Office Annual Review Conference, Wake Forest University, Winston-Salem, NC.
10. **K. Biswas** (2016) “Emerging New Ternary Halides as Scintillators for Radiation Detection”, IEEE Nuclear Science Symposium and Medical Imaging Conference, Strasbourg, France.
11. B. Kang and **K. Biswas** (2016) “Cesium Hafnium Chloride (CHC): Scintillator for Gamma Spectroscopy”, IEEE Symposium on Radiation Measurements and Applications, University of California, Berkeley, CA.
12. **K. Biswas** and B. Kang (2016) “Ternary and Quaternary Monoclinic Iodides as Scintillators for Radiation Detection”, IEEE Symposium on Radiation Measurements and Applications, University of California, Berkeley, CA.
13. C. Summers, M. Tuck, Q. Feng, B. Kang, and **K. Biswas** (2016) “Electronic Properties of Stable AB<sub>3</sub> Compounds: First-Principles Study”, Domestic Nuclear Detection Office Annual Review Conference, Georgia Institute of Technology, Atlanta, GA.
14. **K. Biswas**, B. Kang, Q. Feng, and C. Summers (2016) “Ternary Halides Emerging as Potential Scintillators”, Domestic Nuclear Detection Office Annual Review Conference, Georgia Institute of Technology, Atlanta, GA.