

Khamala O. Bethuel

CONTACT INFORMATION

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EDUCATION

The University of Texas at El Paso, El Paso, TX, USA.

PhD Candidate., Computational Materials Science, August, 2014 - August, 2018

- Dissertation Topic: "Structural and Electronic Properties of Methylammonium lead iodide ($\text{CH}_3\text{NH}_3\text{PbI}_3$)/Fullerene or PCBM Interface". We used sophisticated computational Techniques in predicting and developing materials with properties that meet sufficient, clean, sustainable, and efficient energy supply to our world.
- Advisor: Professor **Rajendra Zope**.

Southern University and A & M College Baton Rouge, Baton Rouge, LA

M.S., Material Physics and Mathematics, August, 2014

- Thesis Topic: "Accurate, Calculated Electronic, Transport, and Structural Properties of Zinc-blende and Wurtzite Zinc Sulphide (ZnS)."
- Advisor: Professor **Diola Bagayoko**

LA-SiGMA "**Online Teaching Institute**", LSU-Shreveport. Best Practice in Scientific Teaching in STEM. Instructor: Professor **CYNTHIA J. SISSON**. Summer 2012.

University of Eldoret (Moi University), Eldoret, Kenya.

M.Sc, Physics, December, 2006.

B.Sc, Physics and Mathematics, December, 2005.

WORK EXPERIENCE

Research Experience

The University of Texas at El Paso, El Paso, TX

Research work

August 2014 – Present

Methylammonium lead iodide(perovskite), $\text{CH}_3\text{NH}_3\text{PbI}_3$, is one of the cheapest and environmentally friendly organic-inorganic hybrid perovskite with outstanding performance in photovoltaic applications. I develop perovskite/metallofullerene interfaces that have excellent properties for solar cells and medical applications such as X-ray contrast imaging. I use several open source software packages in designing the interface then carry out simulations to determine the strongest binding sites at their ground state level. To this far, we have already determined interfaces with excellent charge carrier transport that can develop perovskite solar cells with over 22 percent solar power conversion efficiencies. Most conventional solar cells have less than 20 percent efficiency. The outstanding interfacial characteristics for the most stable structures can be used as guiding principles in the fabrication and design of perovskite solar cells thus addressing energy demands and medical industry needs such as in MRI, X-ray, among others. This work is Directed by Dr. Zope .

Southern University and A & M College, Baton Rouge, LAResearch Assistant**June 2012 – August 2014**

- My research focus on computing physical properties of materials such as II-VI and III-V from first principles. My computational approach follows the Bagayoko, Zhao, and William, and Ekuma and Franklin algorithm (BZW-EF) while adhering to the conventions of state-of-the-art DFT. We successfully combined both algorithms, the methodical code that successfully gives excellent results that match the experiments. Most of the researchers, as evidenced in our citations, have already followed our method into validating their results. This approach plays a crucial role in developing new and unique materials with excellent electrical, transport, and structural properties. The industries thus utilize my already optimized dimensions (properties) to fabricate the novel materials thus avoiding the trial-and error experimental techniques hence economical in terms of time and cost .

TEACHING
EXPERIENCE**El Paso Community College, El Paso, TX, USA.**Adjunct Professor**January 2016 – Present**

- Taught several Physics, Astronomy, and Engineering (Both Lecture and corresponding Laboratories).
- Mentored several students and supervised their research projects.
- Students got highly motivated and realized significant improvement as reflected in their reviews.

ADDITIONAL
TEACHING
EXPERIENCE

- **Lecturer**
Sang'alo Institute of Science and Technology. Bungoma, Kenya. **2007 to 2012**
- **Teacher**
St. Peters Musikoma High School. Bungoma, Kenya. **Aug 2007- May 2012.**
- **Teacher**
St. Martin's Mwibale High School. Bungoma, Kenya. **April 2005- April 2006.**
- **Graduate Assistant** Moi University. Eldoret, Kenya. **2005- 2006**

COMPUTATIONAL
SKILLS

- C/C++, Python, Matlab

SOFTWARE
PACKAGES

- FeniCs, VASP, NRMOL, gromacs, several plotting and visualization packages

PUBLICATIONS

- [1] **B. Khamala**, A. Stewart, L. Franklin, C. E. Ekuma, G. L. Zhao, Y. Malozovsky, and D. Bagayoko, "**Accurate, Calculated electronic, transport, and structural Properties of zinc-blende Zinc Sulphide**" J. Computational condensed matter, 10.1016/j.cocom.2015.12.001. Jan. 2016.
- [2] Yacouba Issa Diakit, Sibiry D. Traor, Yuriy Malozovsky, **Bethuel Khamala**, Lashounda Franklin, Diola Bagayoko. "**Accurate Electronic, Transport, and Bulk Properties of Gallium Arsenide (GaAs)**". Cond-mat.mtrl-sci. Jan. 2016

- [3] Ifeanyi H Nwigboji, John I Ejembi, Yuriy Malozovsky, Bethuel Khamala, Lashounda Franklin, G Zhao, Chinedu E Ekuma, Diola Bagayoko, "**Ab-initio calculations of electronic and transport properties of wurtzite aluminum nitride (w-AIN)**" Journal of Materials Chemistry and Physics, May 1, 2015, vol 157, p. 80-86. doi:10.1016/j.matchemphys.2015.03.019
- [4] Daniel M. Anderson, Jordan Angel, Chris Breward, Pavel Dubovski, Dean Duffy, Ryan Evans, Zachary Grant, Amy Janett, Jiahua Jiang, **Bethuel Khamala**, Ruowen Liu, Zahra Niroobakhsh10, Thierry Platini, Pejman Sanaei, Lan Zhong, "**MPI 2015 - Flooding in Porous Media**" W.L. Gore and Associates, Inc.
- [5] A. Stewart, **B. Khamala**, D. Hart, Y. Malozovisky and D. Bagayoko, "**Ab-initio Calculations of Electronic, Transport and Bulk Properties of cubic Boron Nitride (zb-BN)**" Journal of Advances in Physics 05/2015;9 (1):2277-2286.
- [6] Yacouba Issa DiakitÃf, Sibiry D. TraorÃf, Yuriy Malozovsky, **Bethuel Khamala**, Lashounda Franklin, Diola Bagayoko. "**Calculated Electronic and Related Properties of Wurtzite and Zinc Blende Gallium Nitride (GaN)**". cond-mat.mtrl-sc. <http://arxiv.org/abs/1410.0984>.
- [7] D. Bagayoko, **B. Khamala**, L. franklin, C. E. Ekuma, G. L. Zhao, Y. Malozovsky, D. Yacouba, A.saliev, "**Density functional theory revisited: The Mathematical and Physical Conditions for the Physical Content of the Eigenvalues**". Bulletin of the American Physical Society, 2014/3/5; (59).
- [8] **B. Khamala**, A. Stewart, L. Franklin, C. E. Ekuma, G. L. Zhao, Y. Malozovsky, and D. Bagayoko, "Ab-initio Calculations of Accurate Electronic Properties of wurzite Zinc Sulphide" (manuscript in preparation).
- CONFERENCE TALKS, WORKSHOPS, AND POSTER PRESENTATIONS
- [9] **Bethuel Khamala**, Tunna Baruah, and Rajendra Zope."Structural and electronic Properties of Methylammonium Lead tri-Iodide/Fullerene" Presented a talk at The Graduate student Research Expo held at Hilton hotel, El Paso, Texas. Nov.09, 2017.
- [10] **Bethuel Khamala**, Tunna Baruah, and Rajendra Zope."Structural and electronic Properties of Methylammonium Lead tri-Iodide/Fullerene" Presented a poster to the External Advisory Board (EAB) of PREM Affiliates held at The University of Texas at El Paso, July 28, 2017.
- [11] MPI 2015 Industrial Workshop, University of Delaware, June 22-26, 2015.
- [12] Graduate Student mathematical Modeling Camp (GSMCM), Rensselaer Polytechnic, June 16-19, 2015.
- [13] Careers and opportunities in industry for Mathematical Scientists, Institute for Mathematics and its Applications (IMA), University of Minnesota, Minneapolis, MN. April 20-22, 2015.
- [14] SMU Finite Element Rodeo, Southern Methodist University, Dallas, Texas. February 27-28, 2015.
- [15] Walter Lynn, Bethuel Khamala, Yuriy Malozovsky, and Diola Bagayoko, "**Accurate Electronic, Transport, and Structural Properties of Disodium Sulfide (Na2S)**" presented at the American Physical society (APS), 2015/3 (1), 15007..
- [16] Careers in Mathematical Sciences: Workshop for Underrepresented Groups, Institute for Mathematics and its Applications (IMA), University of Minnesota, Minneapolis, MN. March 26-28, 2015

- [17] **B. Khamala**, A. Stewart, L. Franklin, Y. Malozovsky, and D. Bagayoko, "**Accurate Computations of Electronic and Transport Properties of zinc-blende Zinc Sulphide**" Poster presented at the 2014 Annual Workshop of The University of Texas at El Paso-New Mexico (UTEP/NM), El Paso, Texas. Nov 1, 2014.
- [18] Ifeanyi Nwigboji, Yuriy Malozovsky, John I Ejembi, **B. Khamala**, Diola Bagayoko "**Calculated electronic and transport properties of wurtzite aluminum nitride**", Louisiana Alliance for Simulation-Guided Materials Application (LASIGMA) technical meeting, Baton Rouge, LA. May 5, 2014.
- [19] **B. Khamala**, A. Stewart, L. Franklin, Y. Malozovsky, and D. Bagayoko, "**Accurate Calculations of Electronic and Transport Properties of zinc-blende Zinc Sulphide**" presented at the American Physical society (APS), Denver, Colorado. March 3-7, 2014
- [20] Yacouba Issa DIAKITE, Sibiry D TRAORE, Yuriy MALOZOVSKY, Bethuel KHAMALA, Lashounda FRANKLIN, Diola BAGAYOKO, "**CALCULS DE PROPRIETES ELECTRONIQUES ET AUTRES DES STRUCTURES HEXAGONALE ET CUBIQUE DU NITRURE DE GALLIUM (GAN)**" Presented at MSAS Bamako, Mali.03-08, 2014.
- [21] **B. Khamala**, A. Stewart, L. Franklin, Y. Malozovsky, and D. Bagayoko, "Accurate Calculations of Electronic and Transport Properties of zinc-blende Zinc Sulphide" presented at the 88th Annual meeting of Louisiana Academy of Science (LAS), LSU - Alexandria, LA. March 8, 2014.
- [22] **B. Khamala**, A. Stewart, L. Franklin, Y. Malozovsky, and D. Bagayoko, "**Computation of the Bulk modulus and Total energy of Zn**" presented at the 2014 National Conference of NAAAS, NAHLS, NANAS, and IAAS at the Crowne plaza, Baton Rouge, LA. February 10-15, 2014.
- [23] **B. Khamala**, L. Franklin, C. E. Ekuma, G. L. Zhao, Y. Malozovsky, A. Stewart, and D. Bagayoko, "**Ab-initio Calculations of Accurate Electronic Properties of materials (zb-ZnS)**" at 2013 LA-SIGMA RII Symposium, Marriott Hotel, Baton Rouge, LA. July 29, 2013.
- [24] **B. Khamala**, L. Franklin, C. E. Ekuma, G. L. Zhao, Y. Malozovsky, A. Stewart, and D. Bagayoko, "**Ab-initio Calculations of Accurate Electronic Properties of materials (w-ZnS)**" Presented a poster at the 2013 Southern University Sustainability conference, Baton Rouge, LA. April 22 to 26, 2013.
- [25] S. Adonnay, **B. Khamala**, L. Franklin, C. E. Ekuma, and D. Bagayoko, "**First Principle Study of Electronic structures of (zb-InAs)**." Adonnay presented a poster at the 2013 Southern University Sustainability conference, Baton Rouge, LA. April 22nd to 26th, 2013.
- [26] **B. Khamala**, L. Franklin, C. E. Ekuma, G. L. Zhao, Y. Malozovsky, A. Stewart, and D. Bagayoko, "**Ab-initio Calculations of Accurate Electronic Properties of materials (zb-ZnS)**." Presented a poster at the Fourth Annual Industry-Academia Collaborative Workshop: Next Generation Energy Technology, Marriott Hotel, Baton Rouge, LA. April 9, 2013.
- [27] S. Adonnay, **B. Khamala**, L. Franklin, C. E. Ekuma, and D. Bagayoko, "**First Principle Study of Electronic structures of (zb-GaAs)**." Adonnay presented a poster at the Fourth Annual Industry-Academia Collaborative Workshop: Next Generation Energy Technology, Marriott Hotel, Baton Rouge, LA. April 9, 2013.

- [28] **B. Khamala**, L. Franklin, C. E. Ekuma, G. L. Zhao, Y. Malozovsky, A. Stewart, and D. Bagayoko, "Ab-initio Calculations of Accurate Electronic Properties of (zb-ZnS)." Presented a Poster at the 87th Annual Meeting of Louisiana Academy of Sciences (LAS) at Grambling State University, Grambling, LA, March. 9, 2013.
- [29] A. Stewart, **B. Khamala**, L. Franklin, C. E. Ekuma, G. L. Zhao, Y. Malozovsky, and D. Bagayoko, "Ab-initio Calculations of Accurate Electronic Properties of (w-CdS)." Stewart presented at the 87th Annual Meeting of Louisiana Academy of Sciences (LAS) at Grambling State University, Grambling, LA, March 9, 2013.
- [30] NNSA Consortium on Fuel Cells at Southern University, BR, LA. March 21-24, 2013.
- [31] S. Adonnay, **B. Khamala**, L. Franklin, C. E. Ekuma, and D. Bagayoko, "First Principle Study of Electronic structures of (zb-GaAs)." Adonnay presented a poster at the 87th Annual Meeting of Louisiana Academy of Sciences (LAS) at Grambling University, Grambling, LA, March 9, 2013.
- [32] 2012 LA-SiGMA RII Symposium, Marriott Hotel, Baton Rouge, LA. July 23, 2012
- [33] Density Functional Theory Workshop Louisiana State University, Baton Rouge, LA. July 23 - 27, 2012.
- [34] Virtual School of Computation Science and Engineering (VSCSE). VSCSE Programming Heterogeneous Parallel Computing Systems Summer School 2012. Louisiana State University.
- [35] Louisiana Alliance for Simulation-Guided Materials Application (LA-SiGMA) Graduate Student Retreat, Tulane University, New Orleans, LA. July 2, 2012.

PROFESSIONAL MEMBERSHIPS

- Society for Industrial and Applied Mathematics (SIAM)
- American Physical Society (APS)
- Member of Pi Mu Epsilon Louisiana beta Chapter
- American Institute of Physics (AIP)

HONORS AND AWARDS

- Institute for Mathematics and its Applications (IMA), University of Minnesota, Minneapolis, MN. April 20-22, 2015. Awarded 700 US\$ for Travel and presentation in Careers and opportunities in industry for Mathematical Scientists Workshop.
- Institute for Mathematics and its Applications (IMA), University of Minnesota, Minneapolis, MN. March 26-28, 2015. Awarded 700 US\$ for Travel and presentation in Careers in Mathematical Sciences: Workshop for Underrepresented Groups.
- Awarded 500 US\$ partly from Computational Science program and from the Research Grant for Travel and presentation to the SMU Finite Element Rodeo, Dallas, Texas. February 27-28, 2015.
- Research Assistantship Award. August 2014 to Present.
- Awarded 1000 US\$ from Alpha Kappa Alpha Education Advancement Foundation Award (AKA-EAF) 2014-2015.
- Awarded First place in Computer Science, Physics, Chemistry, Mathematics and engineering category Presentation competitions on March 8, 2014 at the 88th Annual Meeting of Louisiana Academy of Science (LAS) LSU-Alexandria.
- Awarded 300 US\$ and Certificate of achievement as First place award in the Poster Presentation competition in Advanced materials category, April 2013 at the SU Sustainability conference.
- Awarded First Place award in Poster Presentation Competition at Grambling State Univ., LA. March, 2013.

- Awarded certificate of Excellence in Best Practices in Scientific Teaching in STEM. LSU- Shreveport, LA-SiGMA July 2012.
- Judge, Baton Rouge 2012 Science Fair Award
- Travel Award from Southern University to Present a Poster at Grambling State University, LA. March, 2013.
- Awarded Research Assistantship May, 2012- Aug, 2014 in part by the NSF and the Louisiana Board of Regents, through LA-SiGMA [Award Nos. EPS- 1003897, NSF (2010-15)-RII-SUBR] and NSFHRD-1002541, the US Department of Energy's NNSA (Award No. DE-NA0001861), LaSPACE, and LONI-SUBR under Dr. Diola Bagayoko.

LEADERSHIP
ROLES

- President Society for Industrial and Applied Mathematics (SIAM), University of Texas at El Paso (UTEP) Chapter, May 2018—Present.
- Vice President Society for Industrial and Applied Mathematics (SIAM), University of Texas at El Paso (UTEP) Chapter, May 2015—May 2018.
- Secretary general, African Student Organization (ASO), University of Texas at El Paso (UTEP), May 2016—May 2017
- President, Society of Physics Students, Department of Physics, Southern University and A & M College, Baton Rouge, LA, May 2012— May 2014

OUTREACH
ENGAGEMENTS
AND COMMUNITY
SERVICE

- Manual duty (Sanctuary keeper) at the Redeemed Gospel Church. August 2014 - present.
- Panel Volunteer for 2015 Graduate Student research Expo, November, 13, 2015.
- Data entry Clerk, 2014 Graduate Student research Expo, Hilton Hotel, El Paso, Texas, November, 14, 2014.
- Panel Volunteer for 2014 Graduate Student research Expo, November, 12, 2014.
- Judge, 2013 Annual Science Fair, Mentorship Academy Charter School, BR., LA, November, 21 2013.
- Judge, 2013 Audubon Science Fair, an Elementary Charter School, BR., LA, October, 31 2013.
- Trained two M Sc. Physics students, and a visiting scholar from Mali-Africa in computing the electrical properties of materials using electronic package from the Ames National laboratory. Southern University, BR., LA. Summer 2013.
- Judge, 2012 4th Annual Kenilworth Science Fair, Kenilworth Science & Technology Charter School, BR.,LA.
- Physics Judge, Baton Rouge STEM EXPO 2012, Kenilworth Science & Technology School, BR., LA., 2012.
- Manual duty at the Christ the King Christian Centre Church in Baton rouge. May 2012 to August 2014.
- Usher at the Christ the King Christian Centre Church in Baton rouge. May 2012 to August 2014.

REFEREES

Available on request.