Khadiza Begam

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Ph.D. (Physics) from Kent State University   https://www.linkedin.com/in/khadiza-begam-8505311aa/

Objective

Currently, working as a postdoc at Oak Ridge National Lab, TN. Ph.D. in Physics (focused on quantum chemistry and physical chemistry). As of being able to work with wide range of materials and their consequent quantum (electronic structure-based calculations) to classical level (experimental research) analyzing expertise leaded me to be a potential candidate for scientific challenges where in this course I can simultaneously learn and leverage my knowledge to a new direction.

Education

2016-2023	Ph.D.	Kent State University (Physics)
2016-2021	MA	Kent State University, OH, USA (Physics)
2011-2015	M. Phil	Bangladesh University of Engineering and Technology (BUET) (Physics)
2009-2010	M.S.	Jahangirnagar University, Bangladesh (Physics)
2004-2009	B.Sc.	Jahangirnagar University, Bangladesh (Physics)

PhD Coursework

Classical Electrodynamics I&II, Classical Mechanics, Quantum Mechanics I, II&III, Thermodynamics & Statistical Mechanics, Solid State Physics, Particle Physics (Advanced Nuclear Physics), Quantum Chromodynamics Applications.

B. Sc Coursework

Nuclear Physics, Advanced Nuclear Physics, Optics, Electronics, Electrodynamics, Classical Mechanics, Quantum Mechanics, Solid State Physics, Advance Plasma Physics,
Chemistry I & II, Advance Mathematical Physics I &II.

Research Skills

Computational:
- Neutron crystallography of dynamic nuclear polarization (DNP) techniques to advance computational methods for characterizing proton contributions and interactions at biomolecular active sites.
- Electronic structure calculations: Absorption, Emission and Multiphoton absorption spectra, Inter and Intra-molecular charge transfer, charge transport, quantum tunneling, triplet formation and triplet transfer.

- Programming & Quantum mechanical modeling: Script writing, code development and debugging, Condensed phase calculations design, asymmetric molecular junction (MJ) design, investigate the twisted intramolecular charge transfer reaction, Solvated NMR Implementation.

Experimental:

- Thin Film Deposition: Vapor Deposition using plasma polymerization, Spin & Bar Coating using Ag nano wire. Chemical process: Thermal Deposition, Thermal Compression, Chemical Cross-linking (Grafting and Sulfonation).
- Characterizations: Neutron Activation Analysis (NAA), Polarizing Optical Microscopy (POM), UV/VIS Spectroscopy, BAM (Brewster's Angle Microscopy), SEM, Impedance Measurements, Refractive Index Measurement, XRD, FTIR.

Software & Programming: Qchem, Fortran, C, C++, Bash, Machine Learning, Linux, VMD, IQmol, Avogadro, LabVIEW, ImageJ, Adobe Photoshop, Mathematica, Origin, Latex, Windows, macOS, PowerPoint, Excel.

Academic Research Projects/Experiences

Computational:

- Investigated the triplet properties and singlet-triplet gap (ΔE_{TS}) onto the organic semiconducting OLEDs and TADF materials to improve the device efficiency.
- Studied the triplet formation and antioxidative triplet-triplet energy transfer in the bacterial reaction center (BRC) to design the artificial photosynthesis.
- Fundamental gap and spectral calculations of organic photoredox catalyst (OPC).
- Computational investigation of the twisted intramolecular charge transfer onto OPC to explain the experimental findings and consequent industrial applications.
- Designed the multiphoton absorption spectroscopy (computationally) to see the fundamental working mechanism (reaction) of acridine radical-based OPC.
- Designed the asymmetric molecular junction (Al- Al_2O_3-C_{60}-Al) using organic semiconductor (C_{60}) and Al_2O_3 as the channel material with Al as the electrodes.
- Studied the quantum tunneling through the molecular junction.
- Studied the effect of contact resistance due to the presence of dielectric barrier (Al_2O_3) between the electrode (Al) and bridging molecule (C_{60}).
- Implemented polarizable continuum model (PCM) based NMR code using Screened Range Separated Hybrid (SRSH) functionals.
- Studied the solvated NMR of common industrial materials and organic systems to understand the molecular magnetic contributions and polarity effects.
- Qchem code development, debugging, installation and check-in as parts of contributing new computational facilities for the user.

Experimental:

- Spectroscopic measurement of liquid crystal (LC), and LC+dye mixture samples for optical applications such as optical display, sunglass and so on.
- Designed experimental setup of refractive index measurement for various samples using LabVIEW interfacing based rotating stage.
- Designed a heating system for an experimental setup to investigate temperature dependence of viscous fluid, which was successfully used to address large temperature changes.
- Developed polymer-based proton exchange membranes (PEMs) using polyethylene terephthalate (PET) and chemical cross-linking to improve the proton exchange functionality.
- Investigated optical, electrical, and surface morphological of the PEMs for the hydrogen fuel cell applications.
- Developed natural fiber-based Polymer composites (PVC-jute) for environmentally friendly applications.

Academic Achievements/Fellowship/ Scholarship/Award

Year	Description
2003-07	Board Scholarship for H. S. C. result
2004-07	General Scholarship for B. Sc result
2008-09	General Scholarship for M. Sc result
2011-12	NISCT Fellowship for M. Phil Research
2019	The Best Poster Award in PiNO conference

Professional Services

Postdoctoral Research Associate at ORNL focusing on biomolecular crystallography, with a specific emphasis on dynamic nuclear polarization (DNP) techniques to advance computational methods for characterizing proton contributions and interactions at biomolecular active sites.

Graduate Research Assistant (2019-2021)
Work Summary: The molecular calculations of i) the formation of a twisted intramolecular charge-transfer species and the photo-physical characterization of an organic photoredox catalyst. ii) Anti-oxidative triplet-triplet energy transfer in the Photosynthesis system. iii) The effect and counter effect of triplet formation in BRC for designing the artificial Photosynthesis system. iv) Triplet benchmark study on various OLEDs and TADF materials. v) Implementation of SRSH functional to study the solvated NMR properties.

Graduate Research Assistant (Jun 2020 – May 2021)
Experimental projects with the collaboration of AMLCI & Alpha Micron Institute.
Project summary: Sample preparation and optical measurements of dye (solvated), liquid crystal (LC), and LC+dye mixture. Refractive index measurement of various glass and plastic substrates using the rotating stage. Nano wire coating onto the plastic substrate and their characterizations.

Graduate Teaching Assistant (Aug 2016-May 2019 and 2021-2023)

Worked in the Physics department at Kent State University.
Course Taught: PHY-13021 & 13022 labs, College Physics II, 7 IDEAS THAT SHOOK UNIVERSE.

*Continued MPhil research at INST, BAEC until joined at Kent State University.

Lecturer of Physics (2011-2015)
2013-2015, Savar Model College, Dhaka, Bangladesh
2011-2012, Green University of Bangladesh
Course Taught: College Physics I and II, Optics, Electricity and Magnetism. Phy lab I and II.

Theses

MS
The thesis is titled "Preparation and Characterization of Radiation-Induced Proton Exchange Membranes (PEMs) for Hydrogen Fuel Cell: Effect of low-cost Catalyst." Jahangirnagar University, Bangladesh, 2010.

MPhil
The thesis is titled "Assessment of Contamination and Nutritional Deficiency in Ready-made Baby Foods Available in Local Market Using Neutron Activation Analysis Technique." Bangladesh University of Engineering and Technology, Bangladesh, 2015.

Ph.D.
The thesis is titled "Polarization Consistent Electronic Structure Theory of Photo-Physical Properties." Kent State University, Kent, OH 44240 USA.

Publications & Presentations (Please visit the Google Scholar link below)

https://scholar.google.com/citations?user=c5kjc60AAAAJ&hl=en

[1] Khadiza Begam, et al., *"Antioxidative Triplet Excitation Energy Transfer in Bacterial Reaction Center Using a Screened Range Separated Hybrid Functional"*, K Begam, H Aksu, BD Dunietz, The Journal of Physical Chemistry B (2024).

[2] Khadiza Begam, et al., *"Solvent Dependent Nuclear Magnetic Resonance Molecular Parameters Based on a Polarization Consistent Screened Range Separated Hybrid Density Functional Theory Framework"* J. Chem. Theory Comput. (2022).

[3] Evgeny Epifanovsky, Andrew T. B. Gilbert, Xintian Feng, Joonho Lee, Yuezhi Mao,Narbe Mardirossian, Pavel Pokhilko, Alec F. White, Marc P. Coons, Adrian L. Dempwolff, Zhengting Gan, Diptarka Hait, Paul R. Horn, Leif D. Jacobson, Ilya Kaliman, Jörg Kussmann, Adrian W. Lange, Ka Un Lao, Daniel S. Levine, Jie Liu,Simon C. McKenzie, Adrian F. Morrison, Kaushik D. Nanda, Felix Plasser, Dirk R. Rehn, Marta L. Vidal, Zhi-Qiang You, Ying Zhu, Bushra Alam, Benjamin J. Albrecht, Abdulrahman Aldossary, Ethan Alguire, Josefine H. Andersen, Vishikh Athavale,Dennis Barton, Khadiza Begam, Andrew Behn, Nicole Bellonzi,

Yves A. Bernard, Eric J. Berquist, Hugh G. A. Burton, Abel Carreras, Kevin Carter-Fenk, Romit Chakraborty, Alan D. Chien, Kristina D. Closser, Vale Cofer-Shabica, Saswata Dasgupta, Marc de Wergifosse, Jia Deng, Michael Diedenhofen, Hainam Do, Sebastian Ehlert, Po-Tung Fang, Shervin Fatehi, Qingguo Feng, Triet Friedhoff, James Gayvert, Qinghui Ge, Gergely Gidofalvi, Matthew Goldey, Joe Gomes, Cristina E. González-Espinoza, Sahil Gulania, Anastasia O. Gunina, Magnus W. D. Hanson-Heine, Phillip H. P. Harbach, Andreas Hauser, Michael F. Herbst, Mario Hernández Vera, Manuel Hodecker, Zachary C. Holden, Shannon Houck, Xunkun Huang, Kerwin Hui, Bang C. Huynh, Maxim Ivanov,4,ah) Ádám Jász, Hyunjun Ji, Hanjie Jiang, Benjamin Kaduk, Sven Kähler, Kirill Khistyaev, Jaehoon Kim,Gergely Kis, Phil Klunzinger, Zsuzsanna Koczor-Benda, Joong Hoon Koh, Dimitri Kosenkov, Laura Koulias, Tim Kowalczyk, Caroline M. Krauter, Karl Kue, Alexander Kunitsa, Thomas Kus, István Ladjánszki, Arie Landau, Keith V. Lawler, Daniel Lefrancois, Susi Lehtola, Run R. Li, Yi-Pei Li, Jiashu Liang,Marcus Liebenthal, Hung-Hsuan Lin, You-Sheng Lin, Fenglai Liu, Kuan-Yu Liu, Matthias Loipersberger, Arne Luenser, Aaditya Manjanath, Prashant Manohar, Erum Mansoor, Sam F. Manzer, Shan-Ping Mao, Aleksandr V. Marenich, Thomas Markovich,Stephen Mason, Simon A. Maurer, Peter F. McLaughlin, Maximilian F. S. J. Menger, Jan-Michael Mewes, Stefanie A. Mewes, Pierpaolo Morgante, J. Wayne Mullinax, Katherine J. Oosterbaan, Garrette Paran, Alexander C. Paul, Suranjan K. Paul, Fabijan Pavoˇseviˊc, Zheng Pei, Stefan Prager, Emil I. Proynov, Ádám Rák, Eloy Ramos-Cordoba, Bhaskar Rana, Alan E. Rask, Adam Rettig, Ryan M. Richard, Fazle Rob, Elliot Rossomme, Tarek Scheele, Maximilian Scheurer, Matthias Schneider, Nickolai Sergueev, Shaama M. Sharada, Wojciech Skomorowski, David W. Small, Christopher J. Stein, Yu-Chuan Su, Eric J. Sundstrom, Zhen Tao, Jonathan Thirman, Gábor J. Tornai, Takashi Tsuchimochi, Norm M. Tubman, Srimukh Prasad Veccham,Oleg Vydrov, Jan Wenzel, Jon Witte, Atsushi Yamada, Kun Yao, Sina Yeganeh, Shane R. Yost, Alexander Zech, Igor Ying Zhang, Xing Zhang, Yu Zhang, Dmitry Zuev, Alán Aspuru-Guzik, Alexis T. Bell, Nicholas A. Besley, Ksenia B. Bravaya, Bernard R. Brooks, David Casanova, Jeng-Da Chai, Sonia Coriani, Christopher J. Cramer, György Cserey, A. Eugene DePrince , Robert A. DiStasio, Jr., Andreas Dreuw, Barry D. Dunietz, Thomas R. Furlani, William A. Goddard , Sharon Hammes-Schiffer, Teresa Head-Gordon,Warren J. Hehre, Chao-Ping Hsu, Thomas-C. Jagau, Yousung Jung,39,cb) Andreas Klamt,23,cc) Jing Kong,1,bj) Daniel S. Lambrecht, WanZhen Liang, Nicholas J. Mayhall, William McCurdy, Jeffrey B. Neaton, Christian Ochsenfeld, John A. Parkhill, Roberto Peverati,Vitaly A. Rassolov, Yihan Shao, Lyudmila V. Slipchenko, Tim Stauch, Ryan P. Steele, Joseph E. Subotnik, Alex J. W. Thom, Alexandre Tkatchenko, Donald G. Truhlar, Troy Van Voorhis, Tomasz A. Wesolowski, K. Birgitta Whaley, H. Lee Woodcock , Paul M. Zimmerman, Shirin Faraji, Peter M. W. Gill, Martin Head-Gordon, John M. Herbert, and Anna I. Krylov, "*Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package*", J. Chem. Phys. 155, 084801 (2021).

[4] Khadiza Begam, Srijana Bhandari, Buddhadev Maiti, and Barry D. Dunietz "*Screened Range-Separated Hybrid Functional with Polarizable Continuum Model to Overcome Challenges in Describing Triplet Excitations in the Condensed Phase using TDDFT*", *J. Chem. Theo. Comp.* 16 (5), 3287-3293 (2020).

[5] MacKenzie, Ian A., Wang, Leifeng Nicholas P. R. Onuska, Olivia F. Williams, Khadiza Begam, Andrew M. Moran, Barry D. Dunietz, and David A. Nicewicz "*Discovery and Characterization of Acridine Radical Photo reductants*", Nature 580 (7801), 76-80 (2020).

[6] <u>Khadiza Begam</u>, et al., "*Properties of Proton Exchange Membranes Poly-ethylene Terephthalate (PET) Films Developed Gamma by Radiation Induced Grafting and Sulfonation Technique*", *Phys. Mat. Chem.,* Vol. 1, No. 2, 13-20, (2013).

[7] <u>Khadiza Begam</u>, Mohammad Moshiur Rahman, Mohammad Alamgir Kabir , Umma Tamim, Syed Mohammod Hossain, Afia Begum. "*Natural Radioactivity Level of 238U, 232Th, and 40K in Baby Food and Committed Annual Effective Dose Assessment in Bangladesh*" Int. J. of Env. Moni. and Ana. 8(6): 187-192 (2020).

Conference Presentations (Oral & Posters)

[1] Khadiza Begam, Huseyin Aksu, Budhadev Maiti, Srijana Bhandari, and Barry D. Dunietz, "*Energy and electron transfer from the special pair in the Bacterial Reaction Center (BRC) A computational analysis of the effect of the dielectric environment and structural differences between the two branches*," Polymer Initiative of Northeast Ohio (PiNO) Conference, the best poster, June 2019.

[2] Khadiza Begam, Md. Abul Hossain, Farid Ahmed, Md. Alamgir Kabir, Fahmida Parvin, Jahid M. M. Islam and Mubarak A. Khan "Development of Poly (ethylene terephthalate) based proton exchange membranes (PEMs) and evaluation of the effect of low-cost metals as PEM catalyst", PP28, Bangladesh Chemical Congress 2010.

[3] Khadiza Begam, Md. Abul Hossain, Farid Ahmed, Md. Alamgir Kabir, Fahmida Parvin, Jahid M. M. Islam, and Mubarak A. Khan "*Preparation and Characterization of Gamma Radiation Induced Proton Exchange Membranes (PEMs) for Hydrogen Fuel Cell*," OPC18, Bangladesh Chemical Congress 2010.

[4] Md. Alamgir Kabir, Md. Abul Hossain, Farid Ahmed, Mubarak A. Khan, Md. Tofazzal Hossain, Md. Arifur Rahman, Jahid M. M. Islam, Fahmida Parvin, and Khadiza Begam "*Development and characterization of gelatin/polythiophene (PTEBS) composites for low-cost solar cell applications*," OPC17, Bangladesh Chemical Congress 2010.

[5] Khadiza Begam, Md. Abul Hossain, Farid Ahmed, Md. Alamgir Kabir, Fahmida Parvin, Jahid M. M. Islam and Mubarak A. Khan "*Development of Polymer Based Proton Exchange Membranes (PEMs) and Evaluation of the Effect of Low-Cost Metals as PEM Catalyst for Application of Hydrogen Fuel Cell*," 55. Poster, National Conference on Physics for Development-2011.

References

1. **Dr. Glaser Jens (Postdoctoral Supervisor)**
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   Kent State University, USA.
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   University of Bremen, Germany.
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4. **Dr. Michael Strickland (Chair)**
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