Noor Md Shahriar Khan

+1-334-524-4062 khann@ornl.gov Atlanta, GA Noor Md Shahriar Khan
Shahriar N Khan

Education

PhD **Auburn University**, Computational Chemistry — Aug. 2016 - Dec. 2021
- **Dissertation:** Systematic Characterization of Catalytic Active Sites and Complete Catalytic Cycles for Methane to Methanol Transformation
- **CGPA:** 3.84/4

MS **University of Dhaka**, Applied Chemistry & Chemical Engineering — Jan. 2011 - Apr. 2012
- **Thesis:** Industrial Waste Water Characterization and Treatment using Aquatic Plants
- **CGPA:** 3.24/4

BSc **University of Dhaka**, Applied Chemistry & Chemical Engineering — May 2006 - Oct. 2010
- **Major:** Applied Chemistry
- **CGPA:** 3.46/4

Experience

Georgia Tech, Postdoc Researcher — Atlanta, GA
Jan. 2022 - Nov. 2024
3 years
- Application of DFT based molecular dynamics, QM/MM (Psi4/OpenMM) model to simulate electrochemical reactions with multi-dimensional free-energy calculations
- Study of adsorbents on Pt surface using plane wave DFT calculations
- Coding and data analysis using Python, VMD, Plumed

Los Alamos National Lab, Graduate Intern — Los Alamos, NM
May 2021 - Aug. 2021
3 months
- Characterization of electronic and optical properties of graphene quantum dots (GQDs) utilizing TDDFT
- Modelling of graphene flakes with edge functionalization for enhanced opto-electronic properties

Oak Ridge National Lab, Graduate Intern — Oak Ridge, TN
May 2020 - Aug. 2020
3 months
- Research on structural analysis of the Sulfite reductase and substrate binding with heme and siro-heme complexes
- Collaborated with multiple teams from Oak Ridge National Lab and University of Groningen, The Netherlands, to establish well defined workflow for ADF computational tools

Auburn University, Graduate Research Assistant — Auburn, AL
Aug. 2016 - Dec. 2021
5 years
- Theoretical study of C-H bond activation utilizing quantum mechanical simulations
- Characterization of solvated electrons (ground and excited states) from transition metal-ammonia complexes
- Electronic structures of the ground and excited states of transition metal oxide di-cations (FeO^{2+}, RuO^{2+})
- Scripting, data processing, visualization, and interpretation with Python, Bash, FORTRAN, Origin, GaussView

Technical Expertise

Quantum Chemistry: Density Functional Theory (DFT), Coupled Cluster (CC) Theory, Many-body Perturbation Theory, Multi-reference Methods (CASSCF, MRCI, CASPT2)

Classical/Quantum Molecular Dynamics: Ab Initio Molecular Dynamics (AIMD), Quantum Mechanics based Molecular Dynamics (QM/MM)

Programming Language: Python, FORTRAN

Awards and Fellowships

COSAM Graduate Travel Award: Fall 2021, Auburn University

Outstanding International Graduate Student Award: 2021, Auburn University

Graduate Research and Travel Fellowship: 2020, Auburn University

Graduate Student Council Travel Fellowship: 2020, Auburn University

Selected Talks at Scientific Conferences

Physical Chemistry Divisional Seminar, Auburn University: 2024, Auburn, AL

Spring Symposium, Georgia Institute of Technology: 2024, Atlanta, GA

71st Southeastern Regional Meeting of American Chemical Society: 2021, Birmingham, AL

International Symposium on Molecular Spectroscopy: 2021, Virtual

American Chemical Society Spring Annual Convention: 2021, Virtual

59th Sanibel Symposium: 2019, St. Simons Island, GA

Citation Metrics And Publications

Total Citations: 318 (according to Google Scholar) **h-index:** 09, **i10-index:** 09

1. Khan S. N., Hymel J. H., Pederson J. P., McDaniel J. G.; "Catalytic Role of Methanol in Anodic Coupling Reactions Involving Alcohol Trapping of Cation Radicals", J. Org. Chem., 2024, 89 (24), 18353-18369. 2024

IF: 3.4, Citations: 00

2. Khan S. N., Quebedeaux B., Miliordos E.; "Selective conversion of methane to methanol facilitated by molecular metal–methoxy complexes via a self-correcting chemical cycle", Phys. Chem. Chem. Phys, 2024, 26 (35), 23136-23143. 2024

IF: 3.3, Citations: 00

3. Jackson B. A., Khan S. N., Miliordos E.; "A fresh perspective on metal ammonia molecular complexes and expanded metals: opportunities in catalysis and quantum information", Chem. Commun., 2023, 59, 10572-10587. 2023

IF: 4.9, Citations: 04

4. Hymel J. H., Khan S. N., Pederson J. P., McDaniel J. G.; "Computational Electrosynthesis Study of Anodic Intramolecular Olefin Coupling: Elucidating the Role of the Electrical Double Layer", J. Phys. Chem. C, 2023, 127, 39, 19489–19508. 2023

IF: 3.7, Citations: 03

5. Claveau E. E., Sader S., Jackson B. A., Khan S. N., Miliordos E.; "Transition metal oxide complexes as molecular catalysts for selective methane to methanol transformation: any prospects or time to retire?", Phys. Chem. Chem. Phys., 2023, 25, 5313-5326. 2023

IF: 3.3, Citations: 21

6. Khan S. N., Weight B. M., Gifford B. J., Tretiak S., Bishop A.; "Impact of Graphene Quantum Dot Edge Morphologies on Their Optical Properties", J. Phys. Chem. Lett. 2022, 13, 25, 5801–5807. 2022

IF: 5.7, Citations: 07

7. Khan S. N., Griffith A., De Proft F., Miliordos E., Havenith R. W. A., Bykov D., Cunha A. V.; "[Fe_4S_4] cubane in sulfite reductases: new insights into bonding properties and reactivity", Phys. Chem. Chem. Phys., 2022, 24, 18543-18551. 2022

IF: 3.3, Citations: 02

8. Jordan Z., Khan S. N., Jackson B. A., Miliordos E.; "Can boron form coordination complexes with diffuse electrons? Evidence for linked solvated electron precursors", Electron. Struct., 2022, 4(1), 015001. 2022

IF: 2.6, Citations: 07

9. Khan S. N., Miliordos E.; "Electronic Structure of RhO^{2+}, Its Ammoniated Complexes $(NH_3)_{1\text{-}5}RhO^{2+}$, and Mechanistic Exploration of CH_4 Activation by Them", Inorg. Chem. 2021, 60, 21, 16111–16119. 2021

IF: 4.6, Citations: 06

10. Khan S. N., Miliordos E.; "Scandium in Neutral and Positively Charged Ammonia Complexes: Balancing between Sc^{2+} and Sc^{3+}", J. Phys. Chem. A, 2020, 124, 22, 4400–4412. 2020

IF: 2.9, Citations: 16

11. Khan S. N., Miliordos E.; "Methane to Methanol Conversion Facilitated by Transition-Metal Methyl and Methoxy Units: The Cases of $FeCH_3^+$ and $FeOCH_3^+$", J. Phys. Chem. A, 2019, 123, 26, 5590–5599 2019

IF: 2.9, Citations: 19

12. Khan S. N., Kalemos A., Miliordos E.; "Metal-Free Activation of N2 by Persistent Carbene Pairs: An Ab Initio Investigation", J. Phys. Chem. C, 2019, 123, 35, 21548–21553. 2019

IF: 3.7, Citations: 14

13. Kalemos A., Ariyarathna I. R., Khan S. N., Miliordos E.; "'Hypervalency' and the chemical bond", Comput. Theor. Chem., 2019, 1153, 65-74. 2019

IF: 2.8, Citations: 13

14. Wang M., Khan S. N., Miliordos E., Chen M.; "Enantioselective Allenylation of Aldehydes via Brønsted Acid Catalysis", Adv. Synth. Catal., 2018, 360 (23), 4634-4639. 2018

IF: 5.4, Citations: 53

15. Wang M., Khan S. N., Miliordos E., Chen M.; "Enantioselective Syntheses of Homopropargylic Alcohols via Asymmetric Allenylboration", Org. Lett., 2018, 20, 13, 3810–3814. 2018

IF: 5.2, Citations: 57

16. Kirkland J. K., Khan S. N., Casale B., Miliordos E., Vogiatzis K. D.; "Ligand field effects on the ground and excited states of reactive FeO^{2+} species", Phys. Chem. Chem. Phys., 2018, 20, 28786-28795. 2018

IF: 3.3, Citations: 44

17. Ariyarathna I. R., Khan S. N., Pawłowski F., Ortiz J. V., Miliordos E.; "Aufbau Rules for Solvated Electron Precursors: $Be(NH_3)_4^{0,\pm}$ Complexes and Beyond", J. Phys. Chem. Lett., 2018, 9, 1, 84–88. 2018

IF: 5.7, Citations: 45

18. Khan S. N., Miliordos E.; "The role of $O(^1D)$ in the oxidation mechanism of ethylene by iodosobenzene and other hypervalent molecules", Phys. Chem. Chem. Phys., 2017, 19, 18152-18155. 2017

IF: 3.3, Citations: 07