Shyam Kattel, Ph.D.
Assistant Professor
Department of Physics
University of Central Florida
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Research interests

Computational design of novel materials for clean energy generation/fuel synthesis and energy storage; Thermo/Electro-catalysis; Surface reactions; gas-solid and liquid-solid interfaces.
Methods/Approach: Density functional theory (DFT) electronic structure calculations; Kinetic Monte Carlo (KMC) simulations; Microkinetic modeling and Machine learning

Employment, education and research training

Assistant Professor of Physics; August 2024-present
University of Central Florida, Orlando, FL

Assistant Professor of Physics; Jan 2019-July 2024
Florida A&M University (FAMU), Tallahasssee, FL

Associate Research Scientist; July-Dec 2018
Chemical Engineering, Columbia University, New York, NY

Research Associate; July 2014-June, 2018
Chemical Engineering, Columbia University/Chemistry, Brookhaven National Laboratory (BNL), NY

Postdoctoral Research Associate; August 2012-June, 2014
Materials Science, University of Pittsburgh, Pittsburgh, PA

Ph. D. in Physics; 2012
New Mexico State University (NMSU), Las Cruces, NM

MS in Physics; 2005
Tribhuvan University, Kathmandu, Nepal

BS, Physics; 2001
Mahendra Morang Campus, Biratnagar, Nepal

Awards

Emerging Researcher Award, 2024, FAMU

Dean's Award for Graduate Excellence 2012, College of Arts and Sciences, NMSU

Merit-Based Enhancement Fellowship Award 2011-2012, Graduate School, NMSU

Roberts Memorial Leadership Award 2011, Campus Activities, NMSU

Best Comprehensive Exam Award 2010, Department of Physics, NMSU

Dean's Award for Graduate Excellence 2012, College of Arts and Sciences

Current external grants

1. Perovskite Solar Cell Powered Hydrogen Production Using Low Cost Catalysts, New York State Energy Research and Development Authority (NYSERDA), total funding $400,000 (Kattel portion $85,000), 2024-2025, **Co-PI**

2. Machine Learning Study of Multicomponent Catalysts, Applied Research Institute, UNF/Google $35,000, 2024, **PI**
3. Magnetic Matter at Atomic Pressures, subaward from Laboratory of Laser Energetics, University of Rochester, $530,000, 2023-2028, **Co-PI**
4. Integrated Platform to Predict Degradation of Catalysts for Sustainable Conversion of Alternate Feedstocks to Fuels and Chemicals, DOE, Accelerate Innovations in Emerging Technologies, total funding $8M, (Kattel portion $240,000), 2023-2025, **Co-PI**
5. Electrochemical nitrate reduction to ammonia on single-atom alloy catalysts, DOE (FAIR), $750,000, 2023-2026, **PI.**
6. Excellence in Research: Transition metal carbides and nitrides supported single-atom catalysts for aqueous-phase methanol-reforming, NSF, $650,787, 2022-2025, **PI**.
7. HBCU-RISE: Enhancement of Research and Education Infrastructure in the Chemistry and Engineering of Multifunctional Materials, NSF, $1,000,000, 2022-2025, **Co-PI.**
8. Research Initial Award: A computational study of hydroformylation of ethylene over heterogeneous bimetallic catalysts, NSF, $298,542, 2021-2024, **PI**.

Completed grants

9. Unraveling the Role of Catalytic Surfaces in Planetary Atmospheres, Florida Space Grant, $25,000, 2020, **Co-PI**.

Current external computing time grants

10. National Energy Research Scientific Computing Center (NERSC)
11. Advanced Cyberinfrastructure Coordination Ecosystem: Services & Support (ACCESS)
12. Center of Functional Nanomaterials, Brookhaven National Laboratory (BNL)

Post-doc, graduate, and undergraduate students advised at FAMU

1. Dr. Bipin Lamichhane – Postdoctoral Research Associate (current, FAMU)
2. Dr. Sourav Ghoshal – Postdoctoral Research Associate (current, FAMU)
3. Dr. Adyasa Priyadarsini – Postdoctoral Research Associate (current, FAMU)
4. Debit Subedi – Graduate student (current, FAMU)
5. Chidozie Ezeakunne – Graduate student (current, UCF)

(Past members)

1. Muhammad Jehanzaib Aslam – Graduate Student (FAMU)
2. Michael Lynn – Undergraduate student (2022-2024, FAMU)
3. Ebiere Keniye – Undergraduate student (Summer, 2024, FAMU)
4. Esther Perceval – Undergraduate student (Summer, 2024, FAMU)
5. Emmanual Ray – Undergraduate (Summer 2023, FAMU)
6. Damilola Ologunagba – Graduate student (2019-2022; **graduated with Ph.D.,** FAMU)
7. Fayrachel Peterson- Undergraduate (2021, FAMU)
8. Camillia Fullerton - Undergraduate (2021, FAMU)
9. Elijah Athouris - Undergraduate (2019, FAMU)
10. Liana Vigoa – Undergraduate (2019, FAMU)

Publications (***=**corresponding author; **‡** = co-first author, google scholar citations: 11,000+; h-index = 46)

1. H. Mou, J. J. Jeong, B. Lamichhane, **S. Kattel**, Z, Zhuang, J. H. Lee, Q. Change, J.G. Chen, "Trends in Electrocatalytic activity and stability of transition metal nitrides" *Chem. Catal.*, 2024, 4, 100867.
2. M.S. Kim, B. Lamichhane, J.H. Lee, J.G. Bae, J. Y. Heo, H. J. Lee, **S. Kattel***, J. H. Lee, "Identification and comparison of the local physicochemical structures of transition metal-based layered double hydroxides for high-performance electrochemical oxygen evolution reaction", *J. Energy Chem*., 2023, 87, 89-97.
3. M. Lynn, D. Ologunagba, B. Bangi, **S.Kattel***, "Bulk properties of Transition metal nitrides", *Phys. Chem. Chem. Phys*., 2023, 25, 5156-5163.
4. D. Ologunagba, **S. Kattel***, "A Density Functional Theory Study of Electrochemical Nitrogen Reduction to Ammonia on the (100) Surface of Transition-Metal Oxynitrides", *J. Phys. Chem. C*, 2022, 126, 17045–17055.
5. H. Mou, Q. Chang, Z. Xie, S. Hwang, **S. Kattel***, JG Chen, "Enhancing glycerol electrooxidation from synergistic interactions of platinum and transition metal carbides", *Appl. Catal. B: Environ.*, 2022, 316, 121648.
6. Q. Chang, Y. Liu, J.H. Lee, D. Ologunagba, S. Hwang, Z. Xie, **S. Kattel***, J.H. Lee, J. G. Chen, "Metal-Coordinated Phthalocyanines as Platform Molecules for Understanding Isolated Metal Sites in the Electrochemical Reduction of CO_2", *J. Am. Chem. Soc.*144, 16131-16138.
7. X. Yang, J.H. Lee, **S. Kattel***, B. Xu, J.G. Chen, "Tuning Reaction Pathways of Electrochemical Conversion of CO2 by Growing Pd Shells on Ag Nanocubes", *Nano Lett*, 2022, 22, 4576–4582.
8. D. Ologunagba, **S. Kattel*,** "Pt- and Pd-Modified Transition Metal Nitrides Catalysts for the Hydrogen Evolution Reaction" *Phys. Chem. Chem. Phys.* 2022, 24, 12149-12157. (Back cover)
9. Q. Chang, Y. Hong, H. J. Lee, J. H. Lee, D. Ologunagba, Z. Liang, J. Kim, M. J. Kim, J. W. Hong, L. Song, **S. Kattel***, Z. Chen, J. G. Chen, S.I. Choi, "Achieving complete electrooxidation of ethanol by single atomic Rh decoration of Pt nanocubes" *Proc. Natl. Acad. Sci.* 2022, 119, e2112109119.
10. Q. Chang, J.H. Lee, Y. Liu, Z. Xie, S. Hwang, N.S. Marinkovic, A.H.A. Park, **S. Kattel***, J.G. Chen, "Electrochemical CO_2 Reduction Reaction over Cu Nanoparticles with Tunable Activity and Selectivity Mediated by Functional Groups in Polymeric Binder" *J. Am. Chem. Soc. Au* 2022, 2, 214-222.
11. D. Tian, S.R. Denny, K. Li, H. Wang, **S. Kattel***, J.G. Chen, "Density functional theory studies of transition metal carbides and nitrides as electrocatalysts", *Chem. Soc. Rev*. 2021, 50, 12338-12376.
12. S. Biswas, C. Kundu, A. P. Kulkarni, **S. Kattel**, S. Giddey, S. Bhattacharya, "A Study on CO2 Hydrogenation Using a Ceria–Zirconia Mixed Oxide (CexZr1–xO2)-Supported Fe Catalyst", *Ind. Eng. Chem. Res*. *2021*, 60, 14410–14423.
13. R. Xia, D. Tian, **S. Kattel**, B. Hasa, H. Shin, X. Ma, J.G. Chen, F. Jiao, "Electrochemical reduction of acetonitrile to ethylamine", ***Nat. Commun***. 2021, 12, 1-8.

14. D. Ologunagba, **S. Kattel***, "Transition metal oxynitride catalysts for electrochemical reduction of nitrogen to ammonia", ***Mater. Adv***., 2021, 2, 1263-1270. (Back cover)
15. J.H. Lee, **S. Kattel***, Y. Wang, B.M. Tackett, Z. Xie, S. Hwang, S.R. Denny, W. Xu, J. G. Chen, "Prussian blue analogues as platform materials for understanding and developing oxygen evolution reaction electrocatalysts", ***J. Catal.*** 2021, 393, 390-398.
16. Q. Chang, J. Kim, J. H. Lee, **S. Kattel***, J. G. Chen, S. Choi, Z. Chen, "Boosting Activity and Selectivity of CO_2 Electroreduction by Pre-Hydridizing Pd Nanocubes", ***Small,*** 2021, 16, 2005305.
17. Z. Xie, D. Tian, M. Xie, S.Z. Yang, Y. Xu, N. Rui, J.H. Lee, S.D. Senanayake, K. Li, H. Wang, **S. Kattel***, J.G. Chen "Interfacial Active Sites for CO_2 Assisted Selective Cleavage of C–C/C–H Bonds in Ethane", ***Chem***, 2020, 6, 2703-2716.
18. Z. Xie, Y. Xu, M. Xie, X. Chen, J.H. Lee, E. Stavitski, **S. Kattel***, J.G. Chen "Reactions of CO_2 and ethane enable CO bond insertion for production of C_3 oxygenates", ***Nat. Commun***. 2020, 11, 1-8
19. D. Ologunagba, **S. Kattel*** "Machine Learning Prediction of Surface Segregation Energies on Low Index Bimetallic Surfaces", ***Energies***, 2020, 13, 2182.
20. Q. He, J.H. Lee, D. Liu, Y. Liu, Z. Lin, Z. Xie, S. Hwang, S. **Kattel,*** L. Song,* and J.G. Chen "Accelerating CO_2 Electroreduction to CO Over Pd Single-Atom Catalyst", ***Adv. Funct. Mater****.* 2020, 2000407.
21. B.B. Dangi, **S. Kattel,*** "Growth of carbonaceous material on silicon surface: Case study of 1,3-butadiene molecule", ***Chem. Phys. Lett****.* 2020, 745, 137248.
22. Q. He, D. Liu, J. H. Lee, Y. Liu, Z. Xie, S. Hwang**, S. Kattel,*** L. Song,* and J. G. Chen, "Electrochemical Conversion of CO_2 to Syngas with Controllable CO/H_2 Ratios over Co and Ni Single-Atom Catalysts", ***Angew. Chem. Int. Ed.*** 2020, 59, 3033 – 3037. (Cover)
23. E. Gomez, B. Yan, **S. Kattel**, and J. G. Chen, " Carbon Dioxide Reduction in Tandem with Light Alkane Dehydrogenation" ***Nat. Rev. Chem***., 2019, *3*, 638–649.
24. J. H Lee, **S**. **Kattel‡**, Z. Jiang, Z. Xie, S. Yao, B. M. Tackett, W. Xu, N. S. Marinkovic, and J. G. Chen, "Tuning the Activity and Selectivity of Electroreduction of CO_2 to Synthesis Gas using Bimetallic Catalysts" ***Nat. Commun***, 2019, 10, 3724.
25. Q. Chang, **S. Kattel**, X. Li, Z. Liang, B. Tackett, S. Denny, P. Zhang, D. Su, J. G Chen, Z. Chen, "Enhancing CC Bond Scission for Efficient Ethanol Oxidation using PtIr Nanocube Electrocatalysts", ***ACS Catal.*** 2019, 9, 7618−7625.
26. X. Yang, **S. Kattel‡**, J. Nash, X. Chang, J. H. Lee, Y. Yan, J. G. Chen, B. Xu, "Quantification of Active Sites and Elucidation of Reaction Mechanism of Electrochemical Nitrogen Reduction Reaction on Vanadium Nitride", ***Angew. Chem. Int. Ed.*** 2019, 131, 13906–13910. (Cover)
27. W. W. Luc, B. H. Ko, **S. Kattel**, S. Li, D. Su, J. G. Chen, F Jiao, "SO_2-induced Selectivity Change in CO_2 Electroreduction" ***J. Am. Chem. Soc.*** 2019, 141, 9902-9909.
28. B. Yan, B. Zhao, **S. Kattel**, Q. Wu, S. Yao, D. Su, J. G. Chen, "Tuning CO_2 hydrogenation selectivity via metal-oxide interfacial sites", ***J. Catal.*** 2019, 374, 60-71.

Before joining Florida A & M University

29. J. Wang, **S. Kattel**,‡ C.J. Hawxhurst, J.H. Lee, B.M. Tackett, K. Chang, N. Rui, C. J. Liu, J. G. Chen "Enhancing Activity and Reducing Cost for Electrochemical Reduction of CO_2 by Supporting Palladium on Metal Carbides", ***Angew. Chem. Int. Ed.*** 2019, 58, 6271-6275
30. Y. Wang, **S. Kattel**,‡ W. Gao, K. Li, P. Liu, J. G. Chen, H. Wang, "Exploring the ternary interactions in Cu–ZnO–ZrO_2 catalysts for efficient CO_2 hydrogenation to methanol", ***Nat. Commun.*** 2019, 10, 1166.
31. W. Zhu, **S. Kattel**,‡ F Jiao, J. G. Chen, "Shape-Controlled CO_2 Electrochemical Reduction on Nanosized Pd Hydride Cubes and Octahedra", ***Adv. Energy Mater***. 2019, 9, 1802840.
32. X. Yang, J. Nash, J. Anibal, M. Dunwell, **S. Kattel**, E. Stavitski, K. Attenkofer, J. G. Chen, Y. Yan, and B. Xu, "Mechanistic Insights into Electrochemical Nitrogen Reduction Reaction on Vanadium Nitride Nanoparticles", ***J. Am. Chem. Soc.*** 2018, 140,13387-13391 .
33. J. H. Lee, **S. Kattel**,**‡** Z. Xie, B. M. Tackett, J. Wang, C. J. Liu, and J. G. Chen, "Understanding the Role of Functional Groups in Polymeric Binder for Electrochemical Carbon Dioxide Reduction on Gold Nanoparticles", ***Adv. Funct. Mater.*** 2018, 1804762.
34. K. A. Kuttiyiel, **S. Kattel**, S. Cheng, J. H. Lee, L. Wu, Y. Zhu, G. G. Park, P. Liu, K. Sasaki, J. G. Chen, and R. R. Adzic, "Au-Doped Stable L10 Structured Platinum Cobalt Ordered Intermetallic Nanoparticle Catalysts for Enhanced Electrocatalysis", ***ACS Appl. Energy Mater.*** 2018, 1, 3771−3777.
35. B. Yan, S. Yao, **S. Kattel**, Q. Wu, Z. Xie, E. Gomez, P. Liu, D. Su, and J. G. Chen, "Active sites for tandem reactions of CO_2 reduction and ethane dehydrogenation", ***Proc. Natl. Acad. Sci.*** 2018, 115, 8278-8283.
36. **S. Kattel**, J. G. Chen and P. Liu, "Mechanistic study of dry reforming of ethane by CO_2 on a bimetallic PtNi (111) model surface", ***Catal. Sci. & Technol***. 2018, 8, 3748–3758 (Back cover).
37. J. Wang, S. **Kattel**, Z. Wang, J. G Chen and C.J. Liu, "L-Phenylalanine Templated Platinum Catalyst with Enhanced Performance for Oxygen Reduction Reaction", ***ACS Appl. Mater. & Interfaces***, 2018, 10, 21321−21327.
38. Z. Xie, B. Yan, **S. Kattel**, J. H. Lee, S. Yao, Q. Wu, N. Rui, E. Gomez, Z. Liu, W. Xu, L. Zhang, and J. G. Chen, "Dry reforming of methane over CeO_2-supported Pt-Co catalysts with enhanced activity", ***Appl. Catal. B: Environ.*** 2018, 236, 280–293.
39. R. C. E. Hamlyn, M. Mahapatra, D. C. Grinter, F. Xu, S. Luo, R. M. Palomino, **S. Kattel**, I. Waluyo, P. Liu, D. J. Stacchiola, S. D. Senanayake and J. A. Rodriguez, "Imaging the ordering of a weakly adsorbed two-dimensional condensate: ambient-pressure microscopy and spectroscopy of CO_2 molecules on rutile TiO_2(110)", ***Phys. Chem. Chem. Phys.*** 2018, 20, 13122-13126.
40. E. Gomez, **S. Kattel**, B. Yan, S. Yao, P. Liu, and J. G. Chen, "Combining CO_2 reduction with propane oxidative dehydrogenation over bimetallic catalysts", ***Nat. Commun***, 2018, 9, 1398. (Highlighted in BNL: ChemistryViews, Phy.org)
41. L. Wang, S. Zhu, N. Marinkovic, **S. Kattel**, M. Shao, B. Yang, and J. G. Chen, "Insight into the synergistic effect between nickel and tungsten carbide for catalyzing

urea electrooxidation in alkaline electrolyte", ***Appl. Catal. B: Environ.*** 2018, 232, 365–370.

42. X. Li, B. Yan, S. Yao, **S. Kattel**, J. G. Chen, and T. Wang, "Oxidative Dehydrogenation and Dry Reforming of n-Butane with CO_2 over NiFe Bimetallic Catalysts", ***Appl. Catal. B: Environ.*** 2018, 231, 213–223.
43. B. M. Tackett, W. Sheng, **S. Kattel**, S. Yao, B. Yan, K. A. Kuttiyiel, Q. Wu, and J. G. Chen, "Reducing Iridium Loading in Oxygen Evolution Reaction Electrocatalysts Using Core-Shell Particles with Nitride Cores", ***ACS Catal.*** 2018, 8, 2615-2621.
44. **S. Kattel***, P. Liu and J. G. Chen, "Tuning Selectivity of CO_2 Hydrogenation Reactions at the Metal/Oxide Interface", ***J. Am. Chem. Soc.*** 2017, 139, 9739-9754. (Highlighted in JACS spotlights)
45. **S. Kattel**, P. J. Ramírez, J. G. Chen, J. A. Rodriguez, and P. Liu, "Active Sites for CO_2 Hydrogenation to Methanol on Cu/ZnO Catalysts", ***Science*** 2017, 355, 1296-1299. (News coverage in BNL, ChemistryViews, Phy.org, Daily Mail, Chemical and Engineering News)
46. W. Sheng, **S. Kattel**, S. Yao, B. Yan, C. J. Hawxhurst, Q. Wu, and J. G. Chen, "Electrochemical Reduction of CO_2 to Synthesis Gas with Controlled CO/H_2 Ratios", ***Energy Environ. Sci***. 2017, 10, 1180-1185. (Back cover article)
47. X. Li, W. Wan, **S. Kattel**, J. G. Chen, and T. Wang, "Selective Hydrogenation of Biomass-Derived 2(5H)-Furanone over Pt-Ni and Pt-Co Bimetallic Catalysts: From Model Surfaces to Supported Catalysts", ***J. Catal.*** 2016, 344, 148-156.
48. B. Yan, X. Yang, J. Wan, M. Myint, **S. Kattel**, W. Xu, and J. G. Chen, "Dry Reforming of Ethane and Butane with CO_2 over PtNi/CeO_2 Bimetallic Catalysts", ***ACS Catal.*** 2016, 6, 7283-7292.
49. **S. Kattel**, B. Yan, Y. Yang, J. G. Chen, and P. Liu, "Optimizing Binding Energies of Key Intermediates for CO_2 Hydrogenation to Methanol over Oxide-Supported Copper", ***J. Am. Chem. Soc.*** 2016, 138, 12440-12450.
50. T. Nguyen-Phan, S. Luo, D. Vovchok, J. Llorca, S. Sallis, **S. Kattel**, W. Xu, L. F. J. Piper, D. E. Polyansky, S. D. Senanayake, D. J. Stacchiola, and J. A. Rodriguez, "Three-Dimensional Ruthenium-Doped TiO_2 Sea Urchins for Enhanced Visible-Light-Responsive H_2 Production", ***Phys. Chem. Chem. Phys.*** 2016, 18, 15972-15979.
51. **S. Kattel**, W. Yu, B. Yan, X. Yang, Y. Huang, W. Wan, P. Liu, and J. G. Chen, "CO_2 Hydrogenation over Oxide-Supported PtCo Catalysts: The Role of the Oxide Support in Determining the Product Selectivity", ***Angew. Chem. Int. Ed.*** 2016, 55, 7968-7973. (Selected as Hot Paper).
52. **S. Kattel**, B. Yan, J. G. Chen, and P. Liu, "CO_2 Hydrogenation on Pt, Pt/SiO_2 and Pt/TiO_2: Importance of Synergy between Pt and Oxide Support", ***J. Catal.*** 2016, 343, 115-126.
53. K. Liu, **S. Kattel**, V. Mao, and G. Wang, "Electrochemical and Computational Study of Oxygen Reduction Reaction on Non-Precious Transition Metal/Nitrogen Doped Carbon Nanofibers in Acid Medium", ***J. Phys. Chem. C*** 2016, 120, 1586-1596.
54. M. D. Porosoff, M. Myint, **S. Kattel**, Z. Xie, E. Gomez, P. Liu, and J. G. Chen, "Identifying Different Types of Catalysts for CO_2 Reduction by Ethane through Dry Reforming and Oxidative Dehydrogenation", ***Angew. Chem. Int. Ed.*** 2015, 54, 15501-15505.

55. X. Yang, **S. Kattel**, S. D. Senanayake, J. A. Boscoboinik, X. Nie, J. Graciani, J. A. Rodriguez, P. Liu, D. J. Stacchiola, and J. G Chen, "Low Pressure CO_2 Hydrogenation to Methanol over Gold Nanoparticles Activated on a CeO_x/TiO_2 Interface", ***J. Am. Chem. Soc.*** 2015, 137, 10104-10107.

56. X. Yang, **S. Kattel**, K. Xiong, K. Mudiyanselage, S. Rykov, S. D. Senanayake, J. A. Rodriguez, P. Liu, D. J. Stacchiola, and J. G. Chen, "Direct Epoxidation of Propylene over Stabilized Cu^+ Surface Sites on Titanium- Modified Cu_2O", ***Angew. Chem. Int. Ed.*** 2015, 54, 11946 -11951. (Frontispiece)

57. Y. Zhou, Q. Lu, Z. Zhuang, G. S. Hutchings, **S. Kattel**, Y. Yan, J. G. Chen, J. Q. Xiao, and F. Jiao, "Oxygen Reduction at Very Low Overpotential on Nanoporous Ag Catalysts", ***Adv. Energy Mater.*** 2015, 1500149.

58. M. D. Porosoff, **S. Kattel**, W. Li, P. Liu, and J. G. Chen, "Identifying Trends and Descriptors for Selective CO_2 Conversion to CO over Transition Metal Carbides", ***Chem. Commun.*** 2015, 51, 6988-6991.

59. W. Yuan, Y. Jiang, Y. Wang, **S. Kattel**, Z. Zhang, L.Y. Chou, C. K. Tsung, X. Wei, J. Li, X. Zhang, G. Wang, S. X. Mao, and Z. Zhang, "In Situ Observation of Facet-Dependent Oxidation of Graphene on Platinum in an Environmental TEM", ***Chem. Commun.*** 2015, 51, 350-353.

60. **S. Kattel**, and G. Wang, "Beneficial Compressive Strain for Oxygen Reduction Reaction on Pt(111) Surface", ***J. Chem. Phys.*** 2014, 141, 124713.

61. **S. Kattel**, P. Atanassov, and B. Kiefer, "A Density Functional Theory Study of Oxygen Reduction Reaction on Non-PGM Fe-N_x-C Electrocatalysts", ***Phys. Chem. Chem. Phys.*** 2014, 16, 13800-13806.

62. **S. Kattel**, P. Atanassov, and B. Kiefer, "Density functional Theory Study of the Oxygen Reduction Reaction Mechanism in a BN Co-Doped Graphene Electrocatalyst", ***J. Mater. Chem. A*** 2014, 2, 10273-10279.

63. **S. Kattel**, and G. Wang, "Reaction Pathway for Oxygen Reduction on FeN_4 Embedded Graphene", ***J. Phys. Chem. Lett.*** 2014, 5, 452-456.

64. **S. Kattel**, "Magnetic Properties of 3d Transition Metals (Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, and Zn) and Nitrogen Functionalized Armchair Graphene Nanoribbon", ***RSC Adv.*** 2013, 3, 21110–21117.

65. **S. Kattel**, and G. Wang, "A Density Functional Theory Study of Oxygen Reduction Reaction on Me-N_4 (Me=Fe, Co, or Ni) Clusters between Graphitic Pores", ***J. Mater. Chem. A*** 2013, 1, 10790-10797.

66. **S. Kattel**, Z. Duan, and G. Wang, "Density Functional Theory Study of an Oxygen Reduction Reaction on a Pt_3Ti Alloy Electrocatalyst", ***J. Phys. Chem. C*** 2013, 117, 7107-7113.

67. **S. Kattel**, P. Atanassov, and B. Kiefer, "Catalytic Activity of Co-N_x/C Electrocatalysts for Oxygen Reduction Reaction: A Density Functional Theory Study", ***Phys. Chem. Chem. Phys.*** 2013, 15, 148-153.

68. **S. Kattel**, B. Kiefer, and P. Atanassov, "Density Functional Theory Study of Ni-N_x/C Electrocatalyst for Oxygen Reduction in Alkaline and Acidic Media", ***J. Phys. Chem. C*** 2012, 116, 17378-17383.

69. **S. Kattel**, P. Atanassov, and B. Kiefer, "Stability, Electronic and Magnetic Properties of In-plane Defects in Graphene: A First-Principles Study", ***J. Phys. Chem. C*** 2012, 116, 8161-8166.
70. T. S. Olson, S. Pylypenko, **S. Kattel**, P. Atanassov, and B. Kiefer, "Selectivity of Cobalt-based Non-platinum Oxygen Reduction Catalysts in the Presence of Methanol and Formic Acid", ***J. Phys. Chem. C*** 2010, 114, 15190-15195.

Patent

1. Q. Chang, **S. Kattel**, Z. Chen, J. G. Chen, S.I. Choi Achieving complete electrooxidation of ethanol by single atomic Rh decoration of Pt nanocubes Patent Application number: 2-2004-001684-4 (status: pending)

Presentations

1. Invited department seminar: Physics department, University of South Florida, April 2024
   Title: Computations guided design of novel materials for energy and sustainability
2. Invited: American Chemical Society Spring meeting, March, 2024. New Orleans, LA
   Title: Designing catalysts for electrochemical CO_2 reduction to C1 products
3. Invited: American Chemical Society Spring meeting, March, 2024. New Orleans, LA
   Title: Tuning the selectivity of electrochemical CO_2 reduction reaction
4. Invited department seminar: Chemistry department, University of Texas at San Antonio, September 2023
   Title: Catalysts design guided by theoretical insights
5. Invited: Florida Section of American Chemical Society meeting, June 2023, Tampa,
   Title: Computations Guided Catalysts Design
6. Invited department seminar: Loyola University of Chicago, April 2023
   Title: Computations Guided Catalysts Design
7. Invited: AIChE meeting, Phoenix, AZ, November 2022
   Title: Transition metal nitride-based catalysts for electrochemical nitrogen reduction and hydrogen evolution reactions
8. Invited department seminar: Kennesaw State University in Georgia, Kennesaw, GA, September, 2022
   Title: Computations Guided Materials Design
9. Invited Colloquium: Association of Nepalese Physicst in America, September 2022
   Title: Computations Guided Design of Materials
10. ACS Fall meeting, Chicago, IL, August 2022
    Title: Theoretical study of electrochemical nitrogen reduction and hydrogen evolution reactions on transition metal nitride-based materials
11. Invited: ACS Florida section meeting, Tampa, FL, August 2022
    Title: Machine Learning Study of bulk and surface properties of alloys
12. ACS Florida section meeting, Tampa, FL, August 2022
    Title: Bulk properties of Transition Metal Nitrides: A Density Functional Theory Study
13. Invited department seminar: Tribhuvan University, Kathmandu, Nepal, July 2022
    Title: Theory Guided Materials Design for Catalysis

14. Invited department seminar: Florida A&M University, Department of Physics, January, 2022

    Title: Strategies to Design Materials for Low-Carbon Footprint Production of Energy and Fuels
15. Invited (virtual): Neplase Student Association, New Mexico State University, March, 2021

    Title: Strategies to design materials for low-carbon footprint production of energy and fuels
16. Invited (virtual): Doollitte Institute, Air Force Research Laboratory, February 2021

    Title: Machine Learning method to study heterogeneous surface catalysis
17. ACS Spring meeting (virtual), April, 2021

    Title: Transition Metal Oxynitrides Catalysts for Electrochemical Reduction of Nitrogen to Ammonia
18. Invited: National Renewable Energy Laboratory (NREL), July 2019, Golden, CO

    Title: Computational catalysis research at FAMU
19. Florida Section of ACS meeting, May 2019, Tampa, FL

    Title: Key Steps and Mechanisms of CO2 Hydrogenation on Metal/Oxide Catalysts
20. Invited: ACS Spring Meeting, 2019, April, Orlando, FL

    Title: Key steps and mechanisms of CO2 hydrogenation on metal/oxide catalysts

(Before joining FAMU)

21. Invited: Department Seminar, August 2018, Florida A&M University,
22. Invited: Department Seminar, April 2018, Department of Materials Science and Engineering, Southern University of Science and Technology, Shenzhen, China
23. Invited: Department Seminar, April 2018, Department of Chemical Engineering, Tsinghua University, Beijing, China
24. Invited: ACS Spring meeting 2018, New Orleans, LA
25. Invited: ACS Fall meeting 2017, Washington DC
26. Invited: International Conference on Catalysis and Chemical Engineering, 2017, Baltimore, MD
27. Invited: August 2016, NASA Ames Research Center, Mountain View, CA **(**Division Seminar)
28. Invited: Departmental seminar, Chemistry and Physical Sciences Department, March, 2016, Pace University, NY (Departmental Seminar)
29. ACS Fall meeting, 2015, Boston, MA
30. APS March Meeting, 2013, Baltimore, MD
31. APS March Meeting, 2012, Boston, MA
32. APS March Meeting, 2011, Dallas, TX
33. 218th ECS Meeting, 2010, Las Vegas, NV
34. APS March Meeting, 2010, Portland, OR

Course Taught at FAMU

	Year/Semester	Course	Level	Short

				description
1.	Online course developed	PHY 5226 Classical Dynamics -I	Graduate level	Online lecture course
2.	Online course developed	PHY 5227 Classical Dynamics -II	Graduate level	Online lecture course
3.	Spring 2019, 2023; Fall 2020	PHY 3424: Optics	Upper level undergraduate	Lecture
4.	Spring 2020, 2023, 2024; Fall 2021	PHZ 3114: Math Physics-II	Upper level undergraduate	Lecture
5.	Fall 2019, 2022, 2023; Spring 2021	PHZ 3113: Math Physics-I	Upper level undergraduate	Lecture
6.	Spring 2022	PHY 2048	Lower level undergraduate	Lecture
7.	Fall 2021	PHY 2049	Lower level undergraduate	Lecture
8.	Spring 2021	PHY 2054	Lower level undergraduate	Lecture
8.	Fall 2020	PHY 2053	Lower level undergraduate	Lecture
10.	Summer 2019	PHY 2049 L	Lower level undergraduate	Laboratory
11.	Fall 2019	PHY 2048 L	Lower level undergraduate	Laboratory
12.	Spring 2019, Spring 2020, Spring 2022, Fall 2022,	PHY 2054 L	Lower level undergraduate	Laboratory

Teaching training/courses completed at FAMU

1. Effective Online Teaching Practices, 2021-2022
2. Writing Across the Curriculum Summer Learning Institute (WAC SLI), Summer 2021
3. Planning & Implementing Effective Teaching Strategies (PIETS), Summer 2021
4. Freshmen Centric Certification Initiative Summer Learning Institute (FCCI SLI), Summer 2021
5. Faculty Certification for Teaching Online-003, Summer 2020

University service at FAMU

1. Organizing committee of STEM day (2019).
2. Organizing committee of STEM day (2020-canceled due to COVID).
3. Special committee on tenure and promotion criterion, College of Science and Technology (2020)
4. EP3 physics department review committee (2021)
5. Math tenure-track faculty search committees, multiple positions (2021)
6. Math instructor search committee (2021)

7. Chemistry instructor search committee (2021)
8. University-level physics department review committee (2022)
9. Chair of graduate student Damilola Ologunagba doctoral committee (2019-2022)
10. Member of physics department seminar committee (2022-present)
11. Physics department webpage committee (2022-present)
12. Physics representative for College-wide Curriculum Committee (2022-present)
13. Physics department Chair search committee (2022-present)
14. Industrial and Manufacturing Engineering tenure track faculty search committee (2022-present)
15. CST representative in faculty senate (2022-present)
16. Member of the recruitment committee for graduate students in the physics department (2022-present)
17. Member of the doctoral committee for graduate students George Kurian (2020-2022) and Damilola Dada (2022-current).
18. Member of faculty senate budget sub-committee (2023-present)

Professional Memberships

American Chemical Society

Synergistic Activities

1. **Journal Reviewer (20+ journals):** Nature Catal., Nat. Commun, JACS, ACS Energy Lett., ACS Catal., ACS Applied Mater. & Interfaces, J. Phys. Chem. C, J. Phys. Chem. Lett., Energy & Environ. Sci., Chem. Comm., Nanoscale, J. Mater. Chem. A, Phys. Chem. Chem. Phys., Angew. Chem. Int. Ed. ChemSusChem, ChemCatChem, Appl. Catal. B, iScience, J. Catal., Appl. Surf. Sci.
2. **Grants Reviewer/panel:** Department of Energy**,** National Science Foundation (NSF), American Chemical Society Petroleum Research Fund
3. **Session Chair/Organizer:** Division of Catalysis Science and Technology, American Chemical Society National Meetings
4. **Summer School:** NSF-HBCU/MI Summer School: Computational Modeling of Disordered Materials, June 03-07, 2019, Long Beach, MS
5. **Workshop:** NSF-AAPT New Faculty Workshop, June 24 28, 2019, Baltimore, MD