

CURRICULUM VITAE

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EDUCATION AND TRAINING

B.S. in Physics, 2002: Ho Chi Minh University of Pedagogy, Vietnam

Ph.D in Physics, 2012: University of Central Florida. Thesis Advisor: Prof. Talat S. Rahman

PROFESSIONAL EXPERIENCES

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| 08/2025 – Present | Assistant Professor, Department of Physics, University of Central Florida. |
| 05/2019 – Present | Secondary Joint Appointment, Renewable Energy & Chemical Transformations cluster, University of Central Florida. |
| 08/2024 – 08/2025 | Associate Scientist, Department of Physics, University of Central Florida. |
| 11/2016 – 08/2024 | Assistant Scientist, Department of Physics, University of Central Florida. |
| 05/2012 – 11/2016 | Postdoctoral Associate, Department of Physics, University of Central Florida. |
| 08/2002 – 08/2004 | Lecturer, Department of Physics, Ho Chi Minh City University of Pedagogy, Vietnam. |

SCIENTIFIC PRODUCTIVITY

Publication: more than 80 articles in high impact journals with more than 3000 citations and an h-index of 28. Full list of publications is available at the end of this CV and at <http://goo.gl/oiMKtv>.

Invited presentations: 13

INVITED PRESENTATIONS

1. “Ammonium cations for enhancing hydrogen evolution reaction” T. Panagiotakopoulos, J. Janisch, D. Le, T. S. Rahman, ACS Fall 2025, August 17-21, 2025, Washington, DC.
2. “Modeling the Complexity of Electrochemical Environment with Grand Canonical Density Functional Theory”, APS Global Physics Summit, March 16–21, 2025, Anaheim, CA.
3. “Non-metal cations in electrocatalysis”, ACS Spring 2025 Meeting & Expo, March 23-27, 2025, San Diego, CA.
4. “Leveraging high-performance computing for realistic material simulations,” UCF Research Computing Symposium, October 1, 2024, Orlando, FL.
5. “Harnessing Controlled Imperfections in Energy Material Design,” Interdisciplinary Seminar: Novel Materials for Health, Energy, and Other Applications, February 24, 2025, Orlando, FL.
6. “Ab initio Simulation of Surface Reaction in Electrochemical Environment with Hybrid Solvent Model”, Surface Science Discussion 2024, On-line Seminar, Poznan, Poland, January 09-10, 2024.

7. "DFT aided machine learning interatomic potentials for realistic simulations of low dimensional system", APS March Meeting, Las Vegas, Nevada, March 05-10, 2023
8. "Search for Spin Crossover Complexes for Molecular Device", Symposium on Deep Learning for Materials Research, Spetses, Greece, 5-10 June 2022
9. "Functionalizing MoS₂ with gold nanoparticles for catalytic applications," D. Le, T. Jiang, T. B. Rawal; T. S. Rahman, ACS Spring 2021 National Meeting, Virtual, April 2021.
10. "Role of the interface in activating single-layer MoS₂," Penn Conference in Theoretical Chemistry (PCTC), Philadelphia, PA, August 17-19, 2017.
11. "2D Materials for cost effective catalysts", APS March Meeting, New Orleans, Louisiana, March 12-17, 2017
12. "Tuning Catalytic Property of Single-Layer MoS₂ through Defects and Supports," 2016 FLAVS, Orlando, Florida, March 2-3, 2016.
13. "Tuning Properties of Single-Layer MoS₂ through alloying and defects", ICSFS 17, Rio, Brazil, September 07-11, 2014.

SYNERGETIC ACTIVITIES

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| 2025- | Member of the Committee on Community Activities of the American Chemical Society |
| 2025 | Co-Organizing symposium "CO ₂ Utilization & Upgrading for Net Zero Emission" for ACS National Meeting, Spring 2025 |
| 2025 | Co-Organizing focus session "Advances in modeling chemical dynamics at molecule-metal interfaces" for APS Global Physics Summit 2025 |
| 2023-2024 | Associate member of the Committee on Community Activities of the American Chemical Society |
| 2022 | Co-Organizing focus session "Computational Design and Discovery of Novel Materials" for APS March Meeting 2022 |
| 2021-2025 | Co-Organizing symposium "Electrocatalysis for Sustainable Energy: Fundamental, Applications, & Perspective" for ACS National Meeting, Fall 2021, 2022, 2023, 2024, 2025 |
| 2021-2025 | Organizing Illustrated Poem Contests for K-12 students in Central Florida |
| 2020-2022 | Chair-Elect, Chair, Immediate-past Chair of the ACS Orlando Local Section: Led the Orlando Section to its first ever ChemLuminary Award; Chemist Celebrate Earth Day Coordinator (2021-2023); Developed the website (https://orlandoacs.org) for the Orlando Section; Currently serving as the webmaster; Member of SERMACS2025 Organizing Committee. |
| 2022-2025 | Faculty Advisor of UCF Lambda Phi Epsilon Fraternity |
| 2020-2021 | Led establishment of American Physical Society's Student Chapter at UCF |
| 2020-2025 | Judge for Seminole County Regional Science, Math, and Engineering Fair. 2023 Captain of Chemistry judges. |
| 2019 | Member of local Organizing Committee for the 79 th Physical Electronics Conference |
| 2018 | Co-Organizing a focus session for APS March Meeting 2019 |
| 2013-2023 | Judge at the UCF graduate Research Forum |
| 2015 | Judge for poster competition at the FLAVS/FSM Symposium |
| 2015 | Assisting Rock Lake Middle School Science Fair |

LANGUAGE SPOKEN

Fluent in English, Vietnamese

RESEARCH TOPICS

Computational modeling of chemical reactions at surfaces of materials.

Theory and computational modeling of vibrational, optical, magnetic properties of materials.

Machine-learning aided material simulations and discovery.

Development of computational technique for electrochemistry.

MEMBERSHIPS

American Physical Society (APS)

American Chemical Society (ACS)

LIST OF PUBLICATIONS

1. K. Kumarasinghe, A. Rahman, M. Tomlinson, D. Le, F. Joshua, L. Zhai, and Y. Nakajima, "Enhancement of the superconducting transition temperature due to multiband effect in the topological nodal-line semimetal $\text{Pb}_{1-x}\text{Sn}_x\text{TaSe}_2$," *Physical Review B* **112**, 054504 (2025). DOI:10.1103/hsdq-2tp9
2. N. Kruse, K. Hazeldine, M. Hedevar, C. Groothuis, D. Le, T.S. Rahman, J.V. Lauritsen, and L. Mohrhusen, "Monolayer TiS_2 Nanosheets on Au(111)-Structural Characterization and Effect of Edge Stability for Shape Control," *Small* e06023 (2025). DOI:10.1002/sml.202506023
3. W.K. Chin, T. Komesu, B. Ashraf, Y. Kumar, Y. Miyai, A. Kumar, D. Le, E.F. Schwier, S.-i. Ideta, T.S. Rahman, K. Shimada, and P.A. Dowben, "Commensurate Palladium Adlayer Formation on 2H- MoS_2 (0001)," *The Journal of Physical Chemistry C* **129**, 15003-15009 (2025). DOI:10.1021/acs.jpcc.5c02908
4. K. Shi, J. Janisch, Z. Ren, Z. Meng, D. Israel, D. Le, W.E. Kaden, T.S. Rahman, and X. Feng, "Ammonium Cation-Promoted CO_2 Electroreduction on Au in Acidic Media," *Journal of the American Chemical Society* **147**, 23277-23285 (2025). DOI:10.1021/jacs.5c08017
5. N. Brinkmann, D. Austin, B. Ashraf, D. Le, T.S. Rahman, and K. Al-Shamery, "Role of Spectator Species for Amine-Surface Chemistry: Reactions of Amines and Alkenes on Pt(111)," *Journal of the American Chemical Society* **147**, 16964-16971 (2025). DOI:10.1021/jacs.5c00567
6. B. Ashraf, N. Brinkmann, D. Austin, D. Le, K. Al-Shamery, and T.S. Rahman, "Unveiling Coverage-Dependent Interactions of N-Methylaniline with the Pt(111) Surface," *The Journal of Physical Chemistry C* **129**, 6196-6210 (2025). DOI:10.1021/acs.jpcc.4c08116
7. D. Austin, A. Barragan, E.D. Switzer, S. Lois, A. Sarasola, D. Le, T.S. Rahman, and L. Vitali, "Evidence of Au(111) topological states in a kagome analogue lattice and their robustness beyond ultra-low temperatures and defect-free conditions," *Nanoscale* **17**, 12087-12093 (2025). DOI:10.1039/d5nr00229j
8. K. Shi, D. Le, T. Panagiotakopoulos, T.S. Rahman, and X. Feng, "Effect of Ammonium-Based Cations on CO_2 Electroreduction," *ACS Catalysis* **15**, 3647-3659 (2025). DOI:10.1021/acscatal.5c00077
9. T. Jiang, D. Le, K.L. Chagoya, D.J. Nash, R.G. Blair, and T.S. Rahman, "Catalytic reduction of carbon dioxide to methanol over defect-laden hexagonal boron nitride: insights into reaction mechanisms," *J Phys Condens Matter* **37**, (2025). DOI:10.1088/1361-648X/adad2b

10. S. Hong, D. Le, W. Tan, S.H. Xie, F.D. Liu, and T.S. Rahman, "Rate-Determining Steps in CO Oxidation on Pt Single Atom Sites on CeO₂ Surfaces," *Journal of Physical Chemistry C* **128**, 13422-13431 (2024). DOI:10.1021/acs.jpcc.4c00723
11. F. Rezvani, D. Austin, D. Le, T.S. Rahman, and S.L. Tait, "Ligand-Coordinated Pt Single-Atom catalyst facilitates Support-Assisted Water-Gas shift reaction," *Journal of Catalysis* **438**, 115723 (2024). DOI:10.1016/j.jcat.2024.115723
12. T. Jiang, Y. Li, Y. Tang, S. Zhang, D. Le, T.S. Rahman, and F. Tao, "Breaking Continuously Packed Bimetallic Sites to Singly Dispersed on Nonmetallic Support for Efficient Hydrogen Production," *ACS Appl Mater Interfaces* **16**, 21757-21770 (2024). DOI:10.1021/acsami.3c18160
13. J. Shi, D. Le, V. Turkowski, N.U. Din, T. Jiang, Q. Gu, and T.S. Rahman, "Thickness dependence of superconductivity in FeSe films," *The European Physical Journal Plus* **138**, 505 (2023). DOI:10.1140/epjp/s13360-023-04126-7
14. D. Le, "An Explicit-Implicit Hybrid Solvent Model for Grand Canonical Simulations of the Electrochemical Environment," *ChemRxiv* (2023). DOI:10.26434/chemrxiv-2023-z2n4n
15. T. Ekanayaka, T. Jiang, E. Delahaye, O. Perez, J.-P. Sutter, D. Le, A.T. N'Diaye, R. Streubel, T.S. Rahman, and P.A. Dowben, "Evidence of symmetry breaking in a Gd₂ di-nuclear molecular polymer," *Physical Chemistry Chemical Physics* **25**, 6416-6423 (2023). DOI:10.1039/D2CP03050K
16. N.U. Din, D. Le, and T.S. Rahman, "Computational screening of chemically active metal center in coordinated dipyrindyl tetrazine network," *Journal of Physics: Condensed Matter* **35**, (2023). DOI:10.1088/1361-648X/acb8f3
17. E. Mishra, T.K. Ekanayaka, T. Panagiotakopoulos, D. Le, T.S. Rahman, P. Wang, K.A. McElveen, J.P. Phillips, M. Zaid Zaz, S. Yazdani, A.T. N'Diaye, R.Y. Lai, R. Streubel, R. Cheng, M. Shatruk, and P.A. Dowben, "Electronic structure of cobalt valence tautomeric molecules in different environments," *Nanoscale* **15**, 2044-2053 (2023). DOI:10.1039/D2NR06834F
18. D. Le and T.S. Rahman, "On the role of metal cations in CO₂ electrocatalytic reduction," *Nature Catalysis* **5**, 977-978 (2022). DOI:10.1038/s41929-022-00876-2
19. W. Tan, S. Xie, D. Le, W. Diao, M. Wang, K.-B. Low, D. Austin, S. Hong, F. Gao, L. Dong, L. Ma, S.N. Ehrlich, T.S. Rahman, and F. Liu, "Fine-tuned local coordination environment of Pt single atoms on ceria controls catalytic reactivity," *Nature Communications* **13**, 7070 (2022). DOI:10.1038/s41467-022-34797-2
20. E. Wasim, N.U. Din, D. Le, X. Zhou, G.E. Sterbinsky, M.S. Pape, T.S. Rahman, and S.L. Tait, "Ligand-coordination effects on the selective hydrogenation of acetylene in single-site Pd-ligand supported catalysts," *Journal of Catalysis* **413**, 81-92 (2022). DOI:10.1016/j.jcat.2022.06.010
21. J. Koptur-Palenchar, M. Gakiya-Teruya, D. Le, J. Jiang, R. Zhang, X. Jiang, K. Watanabe, T. Taniguchi, H.-P. Cheng, T. Rahman, M. Shatruk, and X.-X. Zhang, "Thickness-dependent spin bistable transitions in single-crystalline molecular 2D material," *npj 2D Materials and Applications* **6**, 59 (2022). DOI:10.1038/s41699-022-00335-3
22. N. Nayyar, D. Le, V. Turkowski, and T.S. Rahman, "Electron-phonon interaction and ultrafast photoemission from doped monolayer MoS₂," *Phys Chem Chem Phys* **24**, 25298-25306 (2022). DOI:10.1039/d2cp02905g

23. T.C. Hung, D. Le, T.S. Rahman, and K. Morgenstern, "Influence of the Moire Pattern of Ag(111)-Supported Graphitic ZnO on Water Distribution," *Journal of Physical Chemistry C* **126**, 12500-12506 (2022). DOI:10.1021/acs.jpcc.2c03274
24. B.T. Blue, S.D. Lough, D. Le, J.E. Thompson, T.S. Rahman, R. Sankar, and M. Ishigami, "Scanning tunneling microscopy and spectroscopy of NiTe₂," *Surface Science* **722**, 122099 (2022). DOI:10.1016/j.susc.2022.122099
25. N.S. Vorobeva, A. Lipatov, A. Torres, J. Dai, J. Abourahma, D. Le, A. Dhingra, S.J. Gilbert, P.V. Galiy, T.M. Nenchuk, D.S. Muratov, T.S. Rahman, X.C. Zeng, P.A. Dowben, and A. Sinitskii, "Anisotropic Properties of Quasi-1D In₄Se₃: Mechanical Exfoliation, Electronic Transport, and Polarization-Dependent Photoresponse," *Advanced Functional Materials* **31**, 2106459 (2021). DOI:10.1002/adfm.202106459
26. K.A.M.H. Siddiquee, R. Munir, C. Dissanayake, X. Hu, S. Yadav, Y. Takano, E.S. Choi, D. Le, T.S. Rahman, and Y. Nakajima, "Fermi surfaces of the topological semimetal CaSn₃ probed through de Haas van Alphen oscillations," *Journal of Physics: Condensed Matter* **33**, 17LT01 (2021). DOI:10.1088/1361-648x/abe0e2
27. T.B. Rawal, D. Le, Z. Hooshmand, and T.S. Rahman, "Toward alcohol synthesis from CO hydrogenation on Cu(111)-supported MoS₂ – predictions from DFT+KMC," *The Journal of Chemical Physics* **154**, 174701 (2021). DOI:10.1063/5.0047835
28. T.W. Morris, D.L. Wisman, N.U. Din, D. Le, T.S. Rahman, and S.L. Tait, "Tailoring the redox capabilities of organic ligands for metal-ligand coordination with vanadium single-sites," *Surface Science* **712**, 121888 (2021). DOI:10.1016/j.susc.2021.121888
29. K. Kuster, Z. Hooshmand, D.P. Rosenblatt, S. Koslowski, D. Le, U. Starke, T.S. Rahman, K. Kern, and U. Schlickum, "Growth of Graphene Nanoflakes/h-BN Heterostructures," *Advanced Materials Interfaces* **8**, 2100766 (2021). DOI:10.1002/admi.202100766
30. T. Jiang, D. Le, T.B. Rawal, and T.S. Rahman, "Syngas molecules as probes for defects in 2D hexagonal boron nitride: their adsorption and vibrations," *Physical Chemistry Chemical Physics* **23**, 7988-8001 (2021). DOI:10.1039/d0cp05943a
31. D. Le, T. Jiang, M. Gakiya-Teruya, M. Shatruk, and T.S. Rahman, "On stabilizing spin crossover molecule [Fe(tBu₂qsal)₂] on suitable supports: insights from ab initio studies," *Journal of Physics: Condensed Matter* **33**, 385201 (2021). DOI:10.1088/1361-648X/ac0beb
32. M. Gakiya-Teruya, X. Jiang, D. Le, Ö. Üngör, A.J. Durrani, J.J. Koptur-Palenchar, J. Jiang, T. Jiang, M.W. Meisel, H.-P. Cheng, X.-G. Zhang, X.-X. Zhang, T.S. Rahman, A.F. Hebard, and M. Shatruk, "Asymmetric Design of Spin-Crossover Complexes to Increase the Volatility for Surface Deposition," *Journal of the American Chemical Society* **143**, 14563-14572 (2021). DOI:10.1021/jacs.1c04598
33. K.L. Chagoya, D.J. Nash, T. Jiang, D. Le, S. Alayoglu, K.B. Idrees, X. Zhang, O.K. Farha, J.K. Harper, T.S. Rahman, and R.G. Blair, "Mechanically Enhanced Catalytic Reduction of Carbon Dioxide over Defect Hexagonal Boron Nitride," *ACS Sustainable Chemistry & Engineering* **9**, 2447-2455 (2021). DOI:10.1021/acssuschemeng.0c06172
34. A. Brooks, T. Jiang, S.L. Liu, D. Le, T.S. Rahman, H.P. Cheng, and X.G. Zhang, "Modeling carrier mobility in graphene as a sensitive probe of molecular magnets," *Physical Review B* **103**, 245423 (2021). DOI:10.1103/PhysRevB.103.245423
35. K. Almeida, K. Chagoya, A. Felix, T. Jiang, D. Le, T.B. Rawal, P.E. Evans, M. Wurch, K. Yamaguchi, P.A. Dowben, L. Bartels, T.S. Rahman, and R.G. Blair, "Methanol carbonylation to acetaldehyde on Au particles supported by single-layer MoS₂ grown on silica," *Journal of Physics: Condensed Matter* **34**, (2021). DOI:10.1088/1361-648X/ac40ad

36. B.T. Young, M.A.K. Pathan, T. Jiang, D. Le, N. Marrow, T. Nguyen, C.E. Jordan, T.S. Rahman, D.M. Popolan-Vaida, and M.E. Vaida, "Catalytic C₂H₂ synthesis via low temperature CO hydrogenation on defect-rich 2D-MoS₂ and 2D-MoS₂ decorated with Mo clusters," *The Journal of Chemical Physics* **152**, 074706 (2020). DOI:10.1063/1.5129712
37. H. Kersell, Z. Hooshmand, G. Yan, D. Le, H. Nguyen, B. Eren, C.H. Wu, I. Waluyo, A. Hunt, S. Nemšák, G. Somorjai, T.S. Rahman, P. Sautet, and M. Salmeron, "CO Oxidation Mechanisms on CoOx-Pt Thin Films," *Journal of the American Chemical Society* **142**, 8312-8322 (2020). DOI:10.1021/jacs.0c01139
38. T. Jiang, D. Le, and T.S. Rahman, "MoS₂-supported Au₃₁ cluster for CO Hydrogenation: A First-Principle Study," *Journal of Vacuum Science & Technology A* **38**, 032201 (2020). DOI:10.1116/1.5142853
39. B.T. Blue, G.G. Jernigan, D. Le, J.J. Fonseca, S.D. Lough, J.E. Thompson, D.D. Smalley, T.S. Rahman, J.T. Robinson, and M. Ishigami, "Metallicity of 2H-MoS₂ induced by Au hybridization," *2D Materials* **7**, 025021 (2020). DOI:10.1088/2053-1583/ab6d34
40. R.S. Berkley, Z. Hooshmand, T. Jiang, D. Le, A.F. Hebard, and T.S. Rahman, "Characteristics of Single-Molecule Magnet Dimers ([Mn₃]₂) on Graphene and h-BN," *The Journal of Physical Chemistry C* **124**, 28186-28200 (2020). DOI:10.1021/acs.jpcc.0c08420
41. S. Posysaev, O. Miroshnichenko, M. Alatalo, D. Le, and T.S. Rahman, "Oxidation states of binary oxides from data analytics of the electronic structure," *Computational Materials Science* **161**, 403-414 (2019). DOI:10.1016/j.commatsci.2019.01.046
42. D.J. Nash, K.L. Chagoya, A. Felix, F.E. Torres-Davila, T. Jiang, D. Le, L. Tetard, T.S. Rahman, and R.G. Blair, "Analysis of the fluorescence of mechanically processed defect-laden hexagonal boron nitride and the role of oxygen in catalyst deactivation," *Advances in Applied Ceramics* **118**, 153-158 (2019). DOI:10.1080/17436753.2019.1584482
43. T.W. Morris, I.J. Huerfano, M. Wang, D.L. Wisman, A.C. Cabelof, N.U. Din, C.D. Tempas, D. Le, A.V. Polezhaev, T.S. Rahman, K.G. Caulton, and S.L. Tait, "Multi-electron Reduction Capacity and Multiple Binding Pockets in Metal-Organic Redox Assembly at Surfaces," *Chemistry - A European Journal* **25**, 5565-5573 (2019). DOI:10.1002/chem.201900002
44. Z. Gao, D. Le, A. Khaniya, C.L. Dezelah, J. Woodruff, R.K. Kanjolia, W.E. Kaden, T.S. Rahman, and P. Banerjee, "Self-Catalyzed, Low-Temperature Atomic Layer Deposition of Ruthenium Metal Using Zero-Valent Ru(DMBD)(CO)₃ and Water," *Chemistry of Materials* **31**, 1304-1317 (2019). DOI:10.1021/acs.chemmater.8b04456
45. R.P. Galhenage, H. Yan, T.B. Rawal, D. Le, A.J. Brandt, T.D. Maddumapatabandi, N. Nguyen, T.S. Rahman, and D.A. Chen, "MoS₂ Nanoclusters Grown on TiO₂ : Evidence for New Adsorption Sites at Edges and Sulfur Vacancies," *Journal of Physical Chemistry C* **123**, 7185-7201 (2019). DOI:10.1021/acs.jpcc.9b00076
46. K. Almeida, P. Pena, T.B. Rawal, W.C. Coley, A.A. Akhavi, M. Wurch, K. Yamaguchi, D. Le, T.S. Rahman, and L. Bartels, "A Single Layer of MoS₂ Activates Gold for Room Temperature CO Oxidation on an Inert Silica Substrate," *Journal of Physical Chemistry C* **123**, 6592-6598 (2019). DOI:10.1021/acs.jpcc.8b12325
47. C.D. Tempas, D. Skomski, B.J. Cook, D. Le, K.A. Smith, T.S. Rahman, K.G. Caulton, and S.L. Tait, "Redox Isomeric Surface Structures Are Preferred over Odd-Electron Pt¹⁺," *Chemistry - A European Journal* **24**, 15852-15858 (2018). DOI:10.1002/chem.201802943
48. C.D. Tempas, T.W. Morris, D.L. Wisman, D. Le, N.U. Ud Din, C.G. Williams, M. Wang, A.V. Polezhaev, T.S. Rahman, K.G. Caulton, and S.L. Tait, "Redox-active Ligand Controlled

- Selectivity of Vanadium Oxidation on Au(100)," *Chemical Science* **9**, 1674-1685 (2018). DOI:10.1039/c7sc04752e
49. T.B. Rawal, S.R. Acharya, S. Hong, D. Le, Y. Tang, F.F. Tao, and T.S. Rahman, "High Catalytic Activity of Pd₁/ZnO(10 $\bar{1}$ 0) toward Methanol Partial Oxidation: A DFT+KMC Study," *ACS Catalysis* **8**, 5553-5569 (2018). DOI:10.1021/acscatal.7b04504
 50. C.S. Merida, D. Le, E.M. Echeverria, A.E. Nguyen, T.B. Rawal, S. Naghibi Alvillar, V. Kandyba, A. Al-Mahboob, Y. Losovyj, K. Katsiev, M.D. Valentin, C.-Y. Huang, M.J. Gomez, I.H. Lu, A. Guan, A. Barinov, T.S. Rahman, P.A. Dowben, and L. Bartels, "Gold Dispersion and Activation on the Basal Plane of Single-Layer MoS₂," *J. Phys. Chem. C* **122**, 267-273 (2018). DOI:10.1021/acs.jpcc.7b07632
 51. P.E. Evans, H.K. Jeong, Z. Hooshmand, D. Le, T.B. Rawal, S. Naghibi Alvillar, L. Bartels, T.S. Rahman, and P.A. Dowben, "Methoxy Formation Induced Defects on MoS₂," *The Journal of Physical Chemistry C* **122**, 10042-10049 (2018). DOI:10.1021/acs.jpcc.8b02053
 52. T.B. Rawal, D. Le, and T.S. Rahman, "MoS₂-supported gold nanoparticle for CO hydrogenation," *Journal of Physics: Condensed Matter* **29**, 415201 (2017). DOI:10.1088/1361-648X/aa8314
 53. T.B. Rawal, D. Le, and T.S. Rahman, "Effect of Single-Layer MoS₂ on the Geometry, Electronic Structure, and Reactivity of Transition Metal Nanoparticles," *The Journal of Physical Chemistry C* **121**, 7282-7293 (2017). DOI:10.1021/acs.jpcc.7b00036
 54. S. Rauschenbach, G. Rinke, R. Gutzler, S. Abb, A. Albarghash, D. Le, T.S. Rahman, M. Durr, L. Harnau, and K. Kern, "Two-Dimensional Folding of Polypeptides into Molecular Nanostructures at Surfaces," *ACS Nano* **11**, 2420-2427 (2017). DOI:10.1021/acsnano.6b06145
 55. M.W. Logan, J.D. Adamson, D. Le, and F.J. Uribe-Romo, "Structural Stability of N-Alkyl-Functionalized Titanium Metal-Organic Frameworks in Aqueous and Humid Environments," *ACS Appl Mater Interfaces* **9**, 44529-44533 (2017). DOI:10.1021/acsami.7b15045
 56. D. Le and T.S. Rahman, "Pt-dipyridyl tetrazine metal-organic network on the Au(100) surface: insights from first principles calculations," *Faraday Discuss* **204**, 83-95 (2017). DOI:10.1039/c7fd00097a
 57. T. Komesu, D. Le, I. Tanabe, E. Schwier, Y. Kojima, M. Zheng, K. Taguchi, M. Koji, T. Okuda, H. Iwasawa, K. Shimada, T.S. Rahman, and P. Dowben, "Adsorbate doping of MoS₂ and WSe₂: the Influence of Na and Co," *Journal of Physics: Condensed Matter* **29**, 285501 (2017). DOI:10.1088/1361-648X/aa7482
 58. Z. Hooshmand, D. Le, and T.S. Rahman, "CO adsorption on Pd(111) at 0.5ML: A first principles study," *Surface Science* **655**, 7-11 (2017). DOI:10.1016/j.susc.2016.09.002
 59. I. Tanabe, T. Komesu, D. Le, T.B. Rawal, E.F. Schwier, M. Zheng, Y. Kojima, H. Iwasawa, K. Shimada, T.S. Rahman, and P.A. Dowben, "The symmetry-resolved electronic structure of 2H-WSe₂(0001)," *Journal of Physics: Condensed Matter* **28**, 345503 (2016). DOI:10.1088/0953-8984/28/34/345503
 60. I. Tanabe, M. Gomez, W.C. Coley, D. Le, E.M. Echeverria, G. Stecklein, V. Kandyba, S.K. Balijepalli, V. Klee, A.E. Nguyen, E. Preciado, I.H. Lu, S. Bobek, D. Barroso, D. Martinez-Ta, A. Barinov, T.S. Rahman, P.A. Dowben, P.A. Crowell, and L. Bartels, "Band structure characterization of WS₂ grown by chemical vapor deposition," *Applied Physics Letters* **108**, 252103 (2016). DOI:10.1063/1.4954278

61. C.J. Páez, K. DeLello, D. Le, A.L.C. Pereira, and E.R. Mucciolo, "Disorder effect on the anisotropic resistivity of phosphorene determined by a tight-binding model," *Physical Review B* **94**, 165419 (2016). DOI:10.1103/PhysRevB.94.165419
62. D.J. Nash, D.T. Restrepo, N.S. Parra, K.E. Giesler, R.A. Penabade, M. Aminpour, D. Le, Z. Li, O.K. Farha, J.K. Harper, T.S. Rahman, and R.G. Blair, "Heterogeneous Metal-Free Hydrogenation over Defect-Laden Hexagonal Boron Nitride," *ACS Omega* **1**, 1343-1354 (2016). DOI:10.1021/acsomega.6b00315
63. J. Katoch, D. Le, S. Singh, R. Rao, T.S. Rahman, and M. Ishigami, "Scattering strength of the scatterer inducing variability in graphene on silicon oxide," *Journal of Physics-Condensed Matter* **28**, 115301 (2016). DOI:10.1088/0953-8984/28/11/115301
64. L.G. AbdulHalim, Z. Hooshmand, M.R. Parida, S.M. Aly, D. Le, X. Zhang, T.S. Rahman, M. Pelton, Y. Losovyj, P.A. Dowben, O.M. Bakr, O.F. Mohammed, and K. Katsiev, "pH-Induced Surface Modification of Atomically Precise Silver Nanoclusters: An Approach for Tunable Optical and Electronic Properties," *Inorganic Chemistry* **55**, 11522–11528 (2016). DOI:10.1021/acs.inorgchem.6b02067
65. E. Ridolfi, D. Le, T.S. Rahman, E.R. Mucciolo, and C.H. Lewenkopf, "A tight-binding model for MoS₂ monolayers," *Journal of Physics: Condensed Matter* **27**, 365501 (2015). DOI:10.1088/0953-8984/27/36/365501
66. A. Ramirez-Torres, D. Le, and T.S. Rahman, "Effect of monolayer supports on the electronic structure of single-layer MoS₂," *IOP Conference Series: Materials Science and Engineering* **76**, 012011 (2015). DOI:10.1088/1757-899x/76/1/012011
67. D. Le, A. Barinov, E. Preciado, M. Isarraraz, I. Tanabe, T. Komesu, C. Troha, L. Bartels, T.S. Rahman, and P.A. Dowben, "Spin-Orbit Coupling in the Band Structure of Monolayer WSe₂," *Journal of Physics: Condensed Matter* **27**, 182201 (2015). DOI:10.1088/0953-8984/27/18/182201
68. J. Mann, Q. Ma, P.M. Odenthal, M. Isarraraz, D. Le, E. Preciado, D. Barroso, K. Yamaguchi, G. von Son Palacio, A. Nguyen, T. Tran, M. Wurch, A. Nguyen, V. Klee, S. Bobek, D. Sun, T.F. Heinz, T.S. Rahman, R. Kawakami, and L. Bartels, "2-Dimensional Transition Metal Dichalcogenides with Tunable Direct Band Gaps: MoS_{2(1-x)}Se_{2x} Monolayers," *Advanced Materials* **26**, 1399-404 (2014). DOI:10.1002/adma.201304389
69. Q. Ma, M. Isarraraz, C.S. Wang, E. Preciado, V. Klee, S. Bobek, K. Yamaguchi, E. Li, P.M. Odenthal, A. Nguyen, D. Barroso, D. Sun, G. von Son Palacio, M. Gomez, A. Nguyen, D. Le, G. Pawin, J. Mann, T.F. Heinz, T.S. Rahman, and L. Bartels, "Post-Growth Tuning of the Bandgap of Single-Layer Molybdenum Disulfide Films by Sulfur/Selenium Exchange," *ACS Nano* **8**, 4672-7 (2014). DOI:10.1021/nn5004327
70. E.A. Lewis, D. Le, A.D. Jewell, C.J. Murphy, T.S. Rahman, and E.C.H. Sykes, "Segregation of Fischer-Tropsch reactants on cobalt nanoparticle surfaces," *Chemical Communications* **50**, 6537-9 (2014). DOI:10.1039/C4CC01680G
71. D. Le, T.B. Rawal, and T.S. Rahman, "Single-Layer MoS₂ with Sulfur Vacancies: Structure and Catalytic Application," *The Journal of Physical Chemistry C* **118**, 5346-5351 (2014). DOI:10.1021/jp411256g
72. T. Komesu, D. Le, X. Zhang, Q. Ma, E.F. Schwier, Y. Kojima, M. Zheng, H. Iwasawa, K. Shimada, M. Taniguchi, L. Bartels, T.S. Rahman, and P.A. Dowben, "Occupied and unoccupied electronic structure of Na doped MoS₂(0001)," *Applied Physics Letters* **105**, 241602 (2014). DOI:10.1063/1.4903824

73. T. Komesu, D. Le, Q. Ma, E.F. Schwier, Y. Kojima, M. Zheng, H. Iwasawa, K. Shimada, M. Taniguchi, L. Bartels, T.S. Rahman, and P.A. Dowben, "Symmetry Resolved Surface-Derived Electronic Structure of MoS₂(0001)," *Journal of Physics: Condensed Matter* **26**, 455501 (2014). DOI:10.1088/0953-8984/26/45/455501
74. Q. Ma, P.M. Odenthal, J. Mann, D. Le, C.S. Wang, Y. Zhu, T. Chen, D. Sun, K. Yamaguchi, T. Tran, M. Wurch, J.L. McKinley, J. Wyrick, K. Magnone, T.F. Heinz, T.S. Rahman, R. Kawakami, and L. Bartels, "Controlled Argon Beam-Induced Desulfurization of Monolayer Molybdenum Disulfide," *Journal of Physics: Condensed Matter* **25**, 252201 (2013). DOI:10.1088/0953-8984/25/25/252201
75. E.A. Lewis, D. Le, A.D. Jewell, C.J. Murphy, T.S. Rahman, and E.C.H. Sykes, "Visualization of Compression and Spillover in a Coadsorbed System: Syngas on Cobalt Nanoparticles," *Acs Nano* **7**, 4384-4392 (2013). DOI:10.1021/nn400919y
76. D. Le, D. Sun, W. Lu, M. Aminpour, C. Wang, Q. Ma, T.S. Rahman, and L. Bartels, "Growth of aligned Mo₆S₆ nanowires on Cu(111)," *Surface Science* **611**, 1-4 (2013). DOI:10.1016/j.susc.2012.12.016
77. D. Le and T.S. Rahman, "Joined edges in MoS₂: metallic and half-metallic wires," *Journal of Physics: Condensed Matter* **25**, 312201 (2013). DOI:10.1088/0953-8984/25/31/312201
78. S. Hong, D. Le, and T. Rahman, "Deactivation of Cu₂O(100) by CO Poisoning," *Topics in Catalysis* **56**, 1082-1087 (2013). DOI:10.1007/s11244-013-0073-7
79. V. Turkowski, S. Babu, D. Le, A. Kumar, M.K. Haldar, A.V. Wagh, Z. Hu, A.S. Karakoti, A.J. Gesquiere, B. Law, S. Mallik, T.S. Rahman, M.N. Leuenberger, and S. Seal, "Linker-induced anomalous emission of organic-molecule conjugated metal-oxide nanoparticles," *ACS Nano* **6**, 4854-4863 (2012). DOI:10.1021/nn301316j
80. D. Sun, W. Lu, D. Le, Q. Ma, M. Aminpour, M. Alcantara Ortigoza, S. Bobek, J. Mann, J. Wyrick, T.S. Rahman, and L. Bartels, "An MoS_x Structure with High Affinity for Adsorbate Interaction," *Angewandte Chemie International Edition* **51**, 10284-10288 (2012). DOI:10.1002/anie.201205258
81. E.A. Lewis, D. Le, C.J. Murphy, A.D. Jewell, M.F.G. Mattera, M.L. Liriano, T.S. Rahman, and E.C.H. Sykes, "Dissociative Hydrogen Adsorption on Close-Packed Cobalt Nanoparticle Surfaces," *Journal of Physical Chemistry C* **116**, 25868-25873 (2012). DOI:10.1021/jp3090414
82. D. Le, D.Z. Sun, W.H. Lu, L. Bartels, and T.S. Rahman, "Single layer MoS₂ on the Cu(111) surface: First-principles electronic structure calculations," *Physical Review B* **85**, 075429 (2012). DOI:10.1103/Physrevb.85.075429
83. D. Le, A. Kara, E. Schroder, P. Hylgaard, and T.S. Rahman, "Physisorption of nucleobases on graphene: a comparative van der Waals study," *Journal of Physics: Condensed Matter* **24**, 424210 (2012). DOI:10.1088/0953-8984/24/42/424210
84. D. Le, M. Aminpour, A. Kiejna, and T.S. Rahman, "The role of van der Waals interaction in the tilted binding of amine molecules to the Au(111) surface," *Journal of physics: Condensed matter* **24**, 222001 (2012). DOI:10.1088/0953-8984/24/22/222001
85. S. Kahle, Z. Deng, N. Malinowski, C. Tonnoir, A. Forment-Aliaga, N. Thontasen, G. Rinke, D. Le, V. Turkowski, T.S. Rahman, S. Rauschenbach, M. Ternes, and K. Kern, "The Quantum Magnetism of Individual Manganese-12-Acetate Molecular Magnets Anchored at Surfaces," *Nano Letters* **12**, 518-521 (2012). DOI:10.1021/nl204141z

86. D. Kim, D. Sun, W. Lu, Z. Cheng, Y. Zhu, D. Le, T.S. Rahman, and L. Bartels, "Toward the growth of an aligned single-layer MoS₂ film," *Langmuir* **27**, 11650–11653 (2011). DOI:10.1021/la201878f
87. D. Sun, D.-H. Kim, D. Le, Ø. Borck, K. Berland, K. Kim, W. Lu, Y. Zhu, M. Luo, J. Wyrick, Z. Cheng, T. Einstein, T. Rahman, P. Hyldgaard, and L. Bartels, "Effective elastic properties of a van der Waals molecular monolayer at a metal surface," *Physical Review B* **82**, 201410 (2010). DOI:10.1103/PhysRevB.82.201410
88. D. Le, S. Stolbov, and T.S. Rahman, "Reactivity of the Cu₂O(100) surface: Insights from first principles calculations," *Surface Science* **603**, 1637-1645 (2009). DOI:10.1016/j.susc.2008.12.039
89. B. White, M. Yin, A. Hall, D. Le, S. Stolbov, T. Rahman, N. Turro, and S. O'Brien, "Complete CO oxidation over Cu₂O nanoparticles supported on silica gel," *Nano Letters* **6**, 2095-8 (2006). DOI:10.1021/nl061457v