

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

- 05/2019 – Present Secondary Joint Appointment, Renewable Energy & Chemical Transformations cluster, University of Central Florida.
- 11/2016 – Present 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 70 articles in high impact journals with more than 3000 citations and an h-index of 24. Full list of publication is available at the end of this CV and at <http://goo.gl/oiMKtv>.

Invited presentations: 8

INVITED PRESENTATIONS

1. “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.
2. “DFT aided machine learning interatomic potentials for realistic simulations of low dimensional system”, APS March Meeting, Las Vegas, Nevada, March 05-10, 2023
3. “Search for Spin Crossover Complexes for Molecular Device”, Symposium on Deep Learning for Materials Research, Spetses, Greece, 5-10 June 2022
4. “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.
5. “Role of the interface in activating single-layer MoS₂,” Penn Conference in Theoretical Chemistry (PCTC), Philadelphia, PA, August 17-19, 2017.
6. “2D Materials for cost effective catalysts”, APS March Meeting, New Orleans, Louisiana, March 12-17, 2017
7. “Tuning Catalytic Property of Single-Layer MoS₂ through Defects and Supports,” 2016 FLAVS, Orlando, Florida, March 2-3, 2016.
8. “Tuning Properties of Single-Layer MoS₂ through alloying and defects”, ICSFS 17, Rio, Brazil, September 07-11, 2014.

SYNERGETIC ACTIVITIES

- 2023-2024 Associate member of the Committee on Community Activities of the American Chemical Society
- 2021-2024 Co-Organizing symposium "Electrocatalysis for Sustainable Energy: Fundamental, Applications, & Perspective" for ACS National Meeting, Fall 2021, 2022, 2023, 2024
- 2022 Co-Organizing focus session "Computational Design and Discovery of Novel Materials" for APS March Meeting 2022
- 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.
- 2022-2023 Faculty Advisor of UCF Lambda Phi Epsilon Fraternity
- 2020-2021 Led establishment of American Physical Society's Student Chapter at UCF
- 2020-2023 Judge for Seminole County Regional Science, Math, and Engineering Fair. 2023 Captain of Chemistry judges.
- 2019 Member of local Organizing Committee for the 79th 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. F. Rezvani, D. Austin, D. Le, T.S. Rahman, and S.L. Tait, "Ligand Coordinated Pt Single-Atom Catalyst Allows Adsorbed CO to Extract Oxygen from the Support During Water-Gas Shift Reaction," **In preparation**, (2024).
2. D. Austin, A. Barragan, E. Switzer, S. Lois, A. Sarasola, D. Le, T. Rahman, and L. Vitali, "Topological states in a pseudo-kagomé lattice," **In preparation**, (2024).

3. 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," **Submitted**, (2024).
4. S. Joshi, D. Le, and T.S. Rahman, "The dynamics of the Si(001) surface: Molecular Dynamics Simulations Using Machine Learning Interatomic Potential," Submitted (2024).
5. K. Shi, D. Le, T. Panagiotakopoulos, T.S. Rahman, and X. Feng, "Effect of Asymmetric Cations on CO₂ Electroreduction," **Submitted to Nature Communication**, (2024).
6. 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 Applied Materials & Interfaces* (2024). DOI:10.1021/acsami.3c18160
7. 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
8. D. Le, "An Explicit-Implicit Hybrid Solvent Model for Grand Canonical Simulations of the Electrochemical Environment," *ChemRxiv* (2023). DOI:10.26434/chemrxiv-2023-z2n4n
9. 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
10. 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
11. 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
12. 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
13. 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
14. 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
15. 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
16. 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

17. 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
18. 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
19. 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
20. 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
21. 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
22. 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
23. 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
24. 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
25. 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
26. 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
27. 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
28. 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
29. 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," *J Phys Condens Matter* **34**, (2021). DOI:10.1088/1361-648X/ac40ad

30. 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
31. 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 CoO_x-Pt Thin Films," *Journal of the American Chemical Society* **142**, 8312-8322 (2020). DOI:10.1021/jacs.0c01139
32. 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
33. 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
34. 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
35. 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
36. 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
37. 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
38. 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
39. 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
40. 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
41. 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
42. 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
43. 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
 44. 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
 45. 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
 46. 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
 47. 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
 48. 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
 49. 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/acsmi.7b15045
 50. 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
 51. 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
 52. 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
 53. 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
 54. 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

55. 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
56. 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
57. 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
58. 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
59. 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
60. 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
61. 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
62. 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
63. 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
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