2021 CINT Publications (342)

1. Abudayyeh, H.; Lubotzky, B.; Blake, A.; Wang, J.; Majumder, S.; Hu, Z.; Kim, Y.; Htoon, H.; Bose, R.; Malko, A. V.; Hollingsworth, J. A.; Rapaport, R. Single Photon Sources with Near Unity Collection Efficiencies by Deterministic Placement of Quantum Dots in Nanoantennas. *Apl Photonics* (2021). DOI:10.1063/5.0034863.
2. Addamane, S. J.; Laurain, A.; Baker, C. W.; Rotter, T. J.; Watt, J.; Reno, J. L.; Balakrishnan, G.; Moloney, J. V. Submonolayer Quantum-Dot Based Saturable Absorber for Femtosecond Pulse Generation. *Journal of Electronic Materials* (2021). DOI: 10.1007/S11664-021-08795-X.
3. Hyder, Ahm G.; Morales, B. A.; Cappelle, M. A.; Percival, S. J.; Small, L. J.; Spoerke, E. D.; Rempe, S.; Walker, W. Evaluation of Electrodialysis Desalination Performance of Novel Bioinspired and Conventional Ion Exchange Membranes with Sodium Chloride Feed Solutions. *Membranes* (2021). DOI: 10.3390/Membranes11030217.
4. Ajantiwalay, T.; Nagel, L.; Maloy, S.; Hattar, K.; Mecholsky Jr, J. J.; Aitkaliyeva, A. Investigation of Hardening Mechanisms and Size Effects in Proton-Irradiated Ht-9 Steels. *Journal of Nuclear Materials* (2021). DOI: 10.1016/J.Jnucmat.2021.152866.
5. Aksoy, D.; Dingreville, R.; Spearot, D. E. Spectrum of Embrittling Potencies and Relation to Properties of Symmetric-Tilt Grain Boundaries. *Acta Materialia* (2021). DOI: 10.1016/J.Actamat.2020.116527.
6. Alberdi, R.; Robbins, J.; Walsh, T.; Dingreville, R. Exploring Wave Propagation in Heterogeneous Metastructures Using the Relaxed Model. *Journal of The Mechanics and Physics of Solids* (2021). DOI: 10.1016/J.Jmps.2021.104540.
7. Alfonso-Hernandez, L.; Oldani, N.; Athanasopoulos, S.; Lupton, J. M.; Tretiak, S.; Fernandez-Alberti, S. Photoinduced Energy Transfer in Linear Guest-Host Chromophores: A Computational Study. *Journal of Physical Chemistry A* (2021). DOI: 10.1021/Acs.Jpca.1c02644.
8. Khalatpour, A.; Paulsen, A. K.; Addamane, S. J.; Deimert, C.; Reno, J. L.; Wasilewski, Z. R.; Hu, Q. A Tunable Unidirectional Source for Gusto's Local Oscillator at 4.74 Thz. *Ieee Transactions on Terahertz Science and Technology* (2021). DOI: 10.1109/Tthz.2021.3124310.
9. Anovitz, L. M.; Affolter, A.; Cheshire, M. C.; Rondinone, A. J.; Allard, L. F. Sol-Gel Synthesis of Nano-Scale, End-Member Albite Feldspar (Naalsi3o8). *Journal of Colloid and Interface Science* (2021). DOI: 10.1016/J.Jcis.2021.06.026.
10. Appelhans, L. N.; Hughes, L.; Mckenzie, B.; Rodriguez, M.; Griego, J.; Briscoe, J.; Moorman, M.; Frederick, E.; Wright, J. B. Facile Microwave Synthesis of Zirconium Metal-Organic Framework Thin Films on Gold and Silicon and Application to Sensor Functionalization. *Microporous and Mesoporous Materials* (2021). DOI: 10.1016/J.Micromeso.2021.111133.
11. Behera, A. K.; Harris, C. T.; Pete, D. V.; Delker, C. J.; Vullum, P. E.; Muniz, M. B.; Koybasi, O.; Taniguchi, T.; Watanabe, K.; Belle, B. D.; Das, S. R. High-Performance and Ultralow-Noise Two-Dimensional Heterostructure Field-Effect Transistors with One-Dimensional Electrical Contacts. *Acs Applied Electronic Materials* (2021). DOI: 10.1021/Acsaelm.1c00595.

12. Lozovoi, A.; Jayakumar, H.; Daw, D.; Vizkelethy, G.; Bielejec, E.; Doherty, M. W.; Flick, J.; Meriles, C. A. Optical Activation and Detection of Charge Transport Between Individual Colour Centres in Diamond. *Nature Electronics* (2021). DOI: 10.1038/S41928-021-00656-Z.

13. Avers, K. E.; Maksimov, P. A.; Rosa, P. F. S.; Thomas, S. M.; Thompson, J. D.; Halperin, W. P.; Movshovich, R.; Chernyshev, A. L. Fingerprinting Triangular-Lattice Antiferromagnet by Excitation Gaps. *Physical Review B* (2021). DOI: 10.1103/physrevb.103.L180406.

14. Baker, J. L.; White, J. T.; Chen, A.; Ulrich, T.; Roback, R. R.; Xu, H. Heat Capacity, Entropy, Formation Energy and Spin-Fluctuation Behavior of U_3si_5 from 2.4 to 397.4 K. *Journal of Nuclear Materials* (2021). DOI: 10.1016/J.Jnucmat.2021.153282.

15. Bandegi, A.; Garcia, M. M.; Banuelos, J. L.; Firestone, M. A.; Foudazi, R. Soft Nanoconfinement of Ionic Liquids in Lyotropic Liquid Crystals. *Soft Matter* (2021). DOI: 10.1039/D1sm00796c.

16. Bandegi, A.; Kim, K.; Foudazi, R. Ion Transport in Polymerized Lyotropic Liquid Crystals Containing Ionic Liquid. *Journal of Polymer Science* (2021). DOI: 10.1002/Pol.20210440.

17. Barr, C. M.; Cooper, M.; Lechman, J.; Bufford, D. C. The Mechanical Response of Micron-Sized Molecular Crystals. *Mrs Advances* (2021). DOI: 10.1557/S43580-021-00124-Y.

18. Barr, C. M.; Foiles, S. M.; Alkayyali, M.; Mahmood, Y.; Price, P. M.; Adams, D. P.; Boyce, B. L.; Abdeljawad, F.; Hattar, K. The Role of Grain Boundary Character in Solute Segregation and Thermal Stability of Nanocrystalline Pt-Au. *Nanoscale* (2021). DOI: 10.1039/D0nr07180c.

19. Baskoro, F.; Wong, H. Q.; Labasan, K. B.; Cho, C.-W.; Pao, C.-W.; Yang, P.-Y.; Chang, C.-C.; Chen, C.-I.; Chueh, C.-C.; Nie, W.; Tsai, H.; Yen, H.-J. An Efficient and Reversible Battery Anode Electrode Derived from a Lead-Based Metal-Organic Framework. *Energy & Fuels* (2021). DOI: 10.1021/Acs.Energyfuels.1c00517.

20. Bates, K. M.; Day, M. W.; Smallwood, C. L.; Owen, R. C.; Schroder, T.; Bielejec, E.; Ulbricht, R.; Cundiff, S. T. Using Silicon-Vacancy Centers in Diamond to Probe the Full Strain Tensor. *Journal of Applied Physics* (2021). DOI: 10.1063/5.0052613.

21. Behzadfar, E.; Kim, K.; Lee, B.; Jordan, A. M.; Lhost, O.; Jaffer, S. A.; Bates, F. S.; Macosko, C. W. Effects of A Layered Morphology on Drip Suppression in Burning Polymers. *Acs Applied Polymer Materials* (2021). DOI: 10.1021/Acsapm.1c00081.

22. Berger Fridman, I.; Ugolini, G. S.; Vandelinder, V.; Cohen, S.; Konry, T. High Throughput Microfluidic System with Multiple Oxygen Levels for The Study of Hypoxia in Tumor Spheroids. *Biofabrication* (2021). DOI: 10.1088/1758-5090/Abdb88.

23. Bhati, M.; Ivanov, S. A.; Senftle, T. P.; Tretiak, S.; Ghosh, D. Nature of Electronic Excitations in Small Non-Stoichiometric Quantum Dots. *Journal of Materials Chemistry A* (2021). DOI: 10.1039/D1ta07983b.

24. Bogan, A.; Studenikin, S.; Korkusinski, M.; Gaudreau, L.; Phoenix, J.; Zawadzki, P.; Sachrajda, A.; Tracy, L.; Reno, J.; Hargett, T. Spin-Orbit Enabled Quantum Transport Channels in A Two-Hole Double Quantum Dot. *Physical Review B* (2021). DOI: 10.1103/Physrevb.103.235310.

25. Bohn, J.; Luk, T. S.; Horsley, S.; Hendry, E. Spatiotemporal Refraction of Light in An Epsilon-

Near-Zero Indium Tin Oxide Layer: Frequency Shifting Effects Arising from Interfaces. *Optica* (2021). DOI: 10.1364/Optica.436324.

26. Bohn, J.; Luk, T. S.; Tollerton, C.; Hutchings, S. W.; Brener, I.; Horsley, S.; Barnes, W. L.; Hendry, E. All-Optical Switching of An Epsilon-Near-Zero Plasmon Resonance in Indium Tin Oxide. *Nature Communications* (2021). DOI: 10.1038/S41467-021-21332-Y.

27. Bonca, J.; Trugman, S. A. Dynamic Properties of a Polaron Coupled to Dispersive Optical Phonons. *Physical Review B* (2021). DOI: 10.1103/Physrevb.103.054304.

28. Brechtl, J.; Agarwal, S.; Hu, X.; Chen, D.; Chancey, M.; Bei, H.; Wang, Y. Q.; Zinkle, S. J. An Exploratory Study on Helium Mobility in Amorphous and Crystallized Bulk Metallic Glasses. *Journal of Nuclear Materials* (2021). DOI: 10.1016/J.Jnucmat.2020.152617.

29. Briggs, S. A.; Steckbeck, M.; Heckman, N. M.; Furnish, T. A.; Bufford, D. C.; Buller, D.; Boyce, B. L.; Hattar, K. A Combined Thermomechanical and Radiation Testing Platform for A 6 Mv Tandem Accelerator. *Nuclear Instruments & Methods in Physics Research Section B-Beam Interactions with Materials and Atoms* (2021). DOI: 10.1016/J.Nimb.2021.08.011.

30. Burns, K.; Bischoff, B.; Barr, C. M.; Hattar, K.; Aitkaliyeva, A. Photo-Exfoliation of Mos_2 Quantum Dots from Nanosheets: An in-Situ Transmission Electron Microscopy Study. *Nanotechnology* (2021). DOI: 10.1088/1361-6528/Ac357c.

31. Burns, K.; Reuel, P. C.; Guerrero, F.; Lang, E.; Lu, P.; Aitkaliyeva, A.; Hattar, K.; Boyle, T. J. Thermal Stability and Radiation Tolerance of Lanthanide-Doped Cerium Oxide Nanocubes. *Crystals* (2021). DOI: 10.3390/Cryst11111369.

32. Bussmann, E.; Butera, R. E.; Owen, J. H. G.; Randall, J. N.; Rinaldi, S. M.; Baczewski, A. D.; Misra, S. Atomic-Precision Advanced Manufacturing for Si Quantum Computing. *Mrs Bulletin* (2021). DOI: 10.1557/S43577-021-00139-8.

33. Campbell, Q.; Ivie, J. A.; Bussmann, E.; Schmucker, S. W.; Baczewski, A. D.; Misra, S. A Model for Atomic Precision P-Type Doping with Diborane on Si(100)-2x1. *Journal of Physical Chemistry C* (2021). DOI: 10.1021/Acs.Jpcc.0c08919.

34. Carr, A.; Bowlan, J.; Mazzoli, C.; Walker, C.; Ding, X.; Barbour, A.; Hu, W.; Wilkins, S.; Kim, J. H.; Lee, N.; Choi, Y. J.; Lin, S.-Z.; Sandberg, R. L.; Zapf, V. S. Dynamics of A Fractal Set of First-Order Magnetic Phase Transitions in Frustrated Lu_2comno_6. *Physical Review B* (2021). DOI: 10.1103/physrevb.103.L060401.

35. Carrasco, R. A.; George, J.; Maestas, D.; Alsaad, Z. M.; Garnham, D.; Morath, C. P.; Duran, J. M.; Ariyawansa, G.; Webster, P. T. Proton Irradiation Effects on Ingaas/Inassb Mid-Wave Barrier Infrared Detectors. *Journal of Applied Physics* (2021). DOI: 10.1063/5.0064043.

36. Carrasco, R. A.; Morath, C. P.; Grant, P. C.; Ariyawansa, G.; Stephenson, C. A.; Kadlec, C. N.; Hawkins, S. D.; Klem, J. F.; Shaner, E. A.; Steenbergen, E. H.; Schaefer, S. T.; Johnson, S. R.; Webster, P. T. Recombination Rate Analysis in Long Minority Carrier Lifetime Mid-Wave Infrared Ingaas/Inassb Superlattices. *Journal of Applied Physics* (2021). DOI: 10.1063/5.0047178.

37. Carroll, J. D.; Exil, A. N.; Dejong, S. A.; Valdez, I. A.; Laursen, C. M.; Deibler, L. A.; Finfrock, C. B.; Boyce, B. L. High-Throughput Statistical Interrogation of Mechanical Properties with Build Plate Location and Powder Reuse in Alsi10 Mg. *Jom* (2021). DOI: 10.1016/J.Jmps.2021.104540.

38. Cazzanelli, M.; Basso, L.; Cestari, C.; Bazzanella, N.; Moser, E.; Orlandi, M.; Piccoli, A.; Miotello, A. Fluorescent Nanodiamonds Synthesized in One-Step by Pulsed Laser Ablation of Graphite in Liquid-Nitrogen. *C-Journal of Carbon Research* (2021). DOI: 10.3390/C7020049.

39. Cetuk, H.; Anishkin, A.; Scott, A. J.; Rempe, S. B.; Ernst, R. K.; Sukharev, S. Partitioning of Seven Different Classes of Antibiotics into Lps Monolayers Supports Three Different Permeation Mechanisms Through the Outer Bacterial Membrane. *Langmuir* (2021). DOI: 10.1021/Acs.Langmuir.0c02652.

40. Chabi, S.; Guler, Z.; Brearley, A. J.; Benavidez, A. D.; Luk, T. S. The Creation of True Two-Dimensional Silicon Carbide. *Nanomaterials* (2021). DOI: 10.3390/Nano11071799.

41. Chaitanya S Deo, E. Y. C. A. R. D. Atomistic Modeling of Radiation Damage in Crystalline Materials.*Modelling and Simulation in Materials Science and Engineering* (2021). DOI: 0.1088/1361-651x/Ac2f83.

42. Chang, C.-C.; Kuo, S.-C.; Cheng, H.-E.; Chen, H.-T.; Yang, Z.-P. Broadband Titanium Nitride Disordered Metasurface Absorbers. *Optics Express* (2021). DOI: 10.1364/Oe.445247.

43. Chang, C.-Y.; Huang, H.-H.; Tsai, H.; Lin, S.-L.; Liu, P.-H.; Chen, W.; Hsu, F.-C.; Nie, W.; Chen, Y.-F.; Wang, L. Facile Fabrication of Self-Assembly Functionalized Polythiophene Hole Transporting Layer for High Performance Perovskite Solar Cells. *Advanced Science* (2021). DOI: 10.1002/Advs.202002718.

44. Chava, V. S. N.; Chandrasekhar, P. S.; Gomez, A.; Echegoyen, L.; Sreenivasan, S. T. Mxene-Based Tailoring of Carrier Dynamics, Defect Passivation, and Interfacial Band Alignment for Efficient Planar P-I-N Perovskite Solar Cells. *Acs Applied Energy Materials* (2021). DOI: 10.1021/Acsaem.1c01669.

45. Chen, A.; Jia, Q. A Pathway to Desired Functionalities in Vertically Aligned Nanocomposites and Related Architectures. *MRS Bulletin* (2021). DOI: 10.1557/S43577-021-00032-4.

46. Chen, D.; Cai, S.; Hsu, N.-W.; Huang, S.-H.; Chuang, Y.; Nielsen, E.; Li, J.-Y.; Liu, C. W.; Lu, T. M.; Laroche, D. Density Dependence of The Excitation Gaps in An Undoped Si/Sige Double-Quantum-Well Heterostructure. *Applied Physics Letters* (2021). DOI: 10.1063/5.0068538.

47. Chen, E. Y.; Hopper, C. P.; Santhapuram, R. R.; Dingreville, R.; Nair, A. K. Origins of The Change in Mechanical Strength of Silicon/Gold Nanocomposites During Irradiation. *Scientific Reports* (2021). DOI: 10.1038/S41598-021-98652-Y.

48. Chen, J.; Jin, Y.; Gao, L.; Reno, J. L.; Kumar, S. Wavelength Beam-Combining of Terahertz Quantum-Cascade Laser Arrays. *Optics Letters* (2021). DOI: 10.1364/Ol.420398.

49. Chen, J. Z.; Talpade, A.; Canning, G. A.; Probus, P. R.; Ribeiro, F. H.; Datye, A. K.; Miller, J. T. Strong Metal-Support Interaction (Smsi) of Pt/Ceo_2 and Its Effect on Propane

Dehydrogenation. *Catalysis Today* (2021). DOI: 10.1016/J.Cattod.2020.06.075.

50. Shang, C.; Wan, Y.; Selvidge, J.; Hughes, E.; Herrick, R.; Mukherjee, K.; Duan, J.; Grillot, F.; Chow, W. W.; Bowers, J. E. Perspectives on Advances in Quantum Dot Lasers and Integration with Si Photonic Integrated Circuits. *Acs Photonics* (2021). DOI: 10.1021/Acsphotonics.1c00707.

51. Choi, J.; Florian, M.; Steinhoff, A.; Erben, D.; Tran, K.; Kim, D. S.; Sun, L.; Quan, J.; Claassen, R.; Majumder, S.; Hollingsworth, J. A.; Taniguchi, T.; Watanabe, K.; Ueno, K.; Singh, A.; Moody, G.; Jahnke, F.; Li, X. Twist Angle-Dependent Interlayer Exciton Lifetimes in Van Der Waals Heterostructures. *Physical Review Letters* (2021). DOI: 10.1103/Physrevlett.126.047401.

52. Chou, K.; Li, N.; Marquis, E. A. Enhanced Work Hardening from Oxygen-Stabilized Omega Precipitates in An Aged Metastable Beta Ti-Nb Alloy. *Acta Materialia* (2021). DOI: 10.1021/Acsami.1c06488.

53. Chow, W. W.; Jahnke, F. Influence of Quantum-Confined Device Fabrication on Semiconductor-Laser Theory. *Journal of Vacuum Science & Technology A* (2021). DOI: 10.1116/6.0000767.

54. Jörg, C.; Vaidya, S.; Noh, J.; Cerjan, A.; Augustine, S.; Von Freymann, G.; Rechtsman, M. C. Observation of Quadratic (Charge-2) Weyl Point Splitting in Near-Infrared Photonic Crystals. *Laser & Photonics Reviews* (2021). DOI: 10.1002/Lpor.202100452.

55. Curwen, C. A.; Addamane, S. J.; Reno, J. L.; Shahili, M.; Kawamura, J. H.; Briggs, R. M.; Karasik, B. S.; Williams, B. S. Thin Thz Qcl Active Regions for Improved Continuous-Wave Operating Temperature. *Aip Advances* (2022). DOI: 10.1063/5.0071953.

56. Clemmer, J. T.; Srivastava, I.; Grest, G. S.; Lechman, J. B. Shear Is Not Always Simple: Rate-Dependent Effects of Flow Type on Granular Rheology. *Physical Review Letters* (2021). DOI: 10.1103/Physrevlett.127.268003.

57. Conway, K. M.; Kunka, C.; White, B. C.; Pataky, G. J.; Boyce, B. L. Increasing Fracture Toughness Via Architected Porosity. *Materials & Design* (2021). DOI: 10.1016/J.Matdes.2021.109696.

58. Cook, R. F.; Boyce, B. L.; Friedman, L. H.; Delrio, F. W. High-Throughput Bend-Strengths of Ultra-Small Polysilicon Mems Components. *Applied Physics Letters* (2021). DOI: 10.1063/5.0049521.

59. Cui, Y.; Aydogan, E.; Gigax, J. G.; Wang, Y.; Misra, A.; Maloy, S. A.; Li, N. in Situ Micro-Pillar Compression to Examine Radiation-Induced Hardening Mechanisms of Fecral Alloys. *Acta Materialia* (2021). DOI: 10.1016/J.Actamat.2020.10.047.

60. Cui, Y.; Derby, B.; Li, N.; Misra, A. Fracture Resistance of Hierarchical Cu-Mo Nanocomposite Thin Films. *Materials Science and Engineering A-Structural Materials Properties Microstructure and Processing* (2021). DOI: 10.1016/J.Msea.2020.139891.

61. Cunningham, W. S.; Hattar, K.; Zhu, Y.; Edwards, D. J.; Trelewicz, J. R. Suppressing Irradiation Induced Grain Growth and Defect Accumulation in Nanocrystalline Tungsten Through Grain

Boundary Doping. *Acta Materialia* (2021). DOI: 10.1016/J.Actamat.2021.116629.

62. Curry, J. F.; Ohta, T.; Delrio, F. W.; Mantos, P.; Jones, M. R.; Babuska, T. F.; Bobbitt, N. S.; Argibay, N.; Krick, B. A.; Dugger, M. T.; Chandross, M. Structurally Driven Environmental Degradation of Friction in Mos_2 Films. *Tribology Letters* (2021). DOI: 10.1007/S11249-021-01453-7.

63. D. Keefer, V. M. F., H. Song, S. Tretiak, S. Fernandez-Alberti, and S. Mukamel. Monitoring Molecular Vibronic Coherences in A Bichromophoric Molecule by Ultrafast X–Ray Spectroscopy. *Chemical Science* (2021). DOI: 10.1039/D0sc06328b.

64. Dennett, C. A.; Dacus, B. R.; Barr, C. M.; Clark, T.; Bei, H.; Zhang, Y.; Short, M. P.; Hattar, K. The Dynamic Evolution of Swelling in Nickel Concentrated Solid Solution Alloys Through in-Situ Property Monitoring. *Applied Materials Today* (2021). DOI: 10.1021/Acs.Chemmater.1c02514.

65. Derby, B. K.; Holesinger, T. G.; Valdez, J. A.; Uberuaga, B. P.; Kreller, C. R. Microstructural Analysis of Novel $Gd_2ti_2o_7$ Thin Films Processed Via Sputter Deposition. *Materials & Design* (2021). DOI:10.1016/J.Matdes.2020.109430.

66. Dingreville, R.; Chen, E. Y.; Deo, C. Temperature and Radiation Effects on Brittle Versus Ductile Fracture Behavior in Miscible Phase Boundaries: Insight from Atomistic Simulations. *International Journal of Fracture* (2021). DOI: 10.1007/S10704-020-00502-X.

67. Dolgopolova, E. A.; Li, D.; Hartman, S. T.; Watt, J.; Rios, C.; Hu, J.; Kukkadapu, R.; Casson, J.; Bose, R.; Malko, A., V; Blake, A., V; Ivanov, S.; Roslyak, O.; Piryatinski, A.; Htoon, H.; Chen, H.-T.; Pilania, G.; Hollingsworth, J. A. Strong Purcell Enhancement at Telecom Wavelengths Afforded by Spinel Fe_3o_4 Nanocrystals with Size-Tunable Plasmonic Properties. *Nanoscale Horizons* (2021). DOI:10.1039/D1nh00497b.

68. Dong, M.; Clark, G.; Leenheer, A. J.; Zimmermann, M.; Dominguez, D.; Menssen, A. J.; Heim, D.; Gilbert, G.; Englund, D.; Eichenfield, M. High-Speed Programmable Photonic Circuits in A Cryogenically Compatible, Visible-Near-Infrared 200 Mm Cmos Architecture. *Nature Photonics* (2021). DOI:10.1038/S41566-021-00903-X.

69. Dub, P. A.; Tkachenko, N., V; Vyas, V. K.; Wills, M.; Smith, J. S.; Tretiak, S. Enantioselectivity in The Noyori-Ikariya Asymmetric Transfer Hydrogenation of Ketones. *Organometallics* (2021). DOI: 10.1021/Acs.Organomet.1c00201.

70. Ducatel, J.; Padawer-Blatt, A.; Bogan, A.; Korkusinski, M.; Zawadzki, P.; Sachrajda, A.; Studenikin, S.; Tracy, L.; Reno, J.; Hargett, T. Single-Hole Couplings in Gaas/Algaas Double Dots Probed with Transport and Edsr Spectroscopy. *Applied Physics Letters* (2021). DOI: 10.1063/5.0044933.

71. Dylan Bardgett, R. N. G., Danielle M. Hamann, Dennice M. Roberts, Sage R. Bauers, Ping Lu, and David C. Johnson. Understanding The Reactions Between Fe and Se Binary Diffusion Couples. *Chemistry of Materials* (2021). DOI: 10.1021/Acs.Chemmater.1c00303.

72. Echeverria, M. J.; Galitskiy, S.; Mishra, A.; Dingreville, R.; Dongare, A. M. Understanding the

Plasticity Contributions During Laser-Shock Loading and Spall Failure of Cu Microstructures at The Atomic Scales. *Computational Materials Science* (2021). DOI: 10.1016/J.Commatsci.2021.110668.

73. Ekanayaka, T. K.; Hao, G.; Mosey, A.; Dale, A. S.; Jiang, X.; Yost, A. J.; Sapkota, K. R.; Wang, G. T.; Zhang, J.; N'diaye, A. T.; Marshall, A.; Cheng, R.; Naeemi, A.; Xu, X.; Dowben, P. A. Nonvolatile Voltage Controlled Molecular Spin-State Switching for Memory Applications. *Magnetochemistry* (2021). DOI: 10.3390/Magnetochemistry7030037.

74. El-Atwani, O.; Alvarado, A.; Unal, K.; Fensin, S.; Hinks, J. A.; Greaves, G.; Baldwin, J. K. S.; Maloy, S. A.; Martinez, E. Helium Implantation Damage Resistance in Nanocrystalline W-Ta-V-Cr High Entropy Alloys. *Materials Today Energy* (2021). DOI: 10.1016/J.Mtener.2020.100599.

75. El-Atwani, O.; Kim, H.; Gigax, J. G.; Harvey, C.; Aytuna, B.; Efe, M.; Maloy, S. A. Stable, Ductile and Strong Ultrafine Ht-9 Steels Via Large Strain Machining. *Nanomaterials* (2021). DOI: 10.1103/Physrevb.104.134306.

76. El-Atwani, O.; Kim, H.; Harvey, C.; Efe, M.; Maloy, S. A. Limitations of Thermal Stability Analysis Via in-Situ Tem/Heating Experiments. *Nanomaterials* (2021). DOI: 10.3390/Nano11102541.

77. Fatima; Inerbaev, T.; Xia, W.; Kilin, D. S. Magnetic-Field-Driven Electron Dynamics in Graphene. *Journal of Physical Chemistry Letters* (2021). DOI: 10.1021/Acs.Jpclett.1c01020.

78. Fauseweh, B.; Zhu, J.-X. Digital Quantum Simulation of Non-Equilibrium Quantum Many-Body Systems. *Quantum Information Processing* (2021). DOI: 10.1007/S11128-021-03079-Z.

79. Fender, S. S.; Thomas, S. M.; Ronning, F.; Bauer, E. D.; Thompson, J. D.; Rosa, P. F. S. Narrow-Gap Semiconducting Behavior in Antiferromagnetic $Eu_{11}insb_9$. *Physical Review Materials* (2021). DOI: 10.1103/Physrevmaterials.5.074603.

80. Frederick, E.; Campbell, Q.; Benavidez, A.; Wheeler, D. R.; Misra, S. Reaction of Dichlorophenylborane with H-Si (100). *Acs Omega* (2021). DOI: 10.1021/Acsomega.1c04619.

81. Frederick, E.; Campbell, Q.; Kolesnichenko, I., V; Pena, L. F.; Benavidez, A.; Anderson, E. M.; Wheeler, D. R.; Misra, S. Ultradoping Boron on Si(100) Via Solvothermal Chemistry. *Chemistry-A European Journal* (2021). DOI: 10.1002/Chem.202102200.

82. Freixas, V. M.; White, A. J.; Nelson, T.; Song, H.; Makhov, D., V; Shalashilin, D.; Fernandez-Alberti, S.; Tretiak, S. Nonadiabatic Excited-State Molecular Dynamics Methodologies: Comparison and Convergence. *Journal of Physical Chemistry Letters* (2021). DOI: 10.1021/Acs.Jpclett.1c00266.

83. Freixas, V. M.; Wilhelm, P.; Nelson, T.; Hinderer, F.; Hoeger, S.; Tretiak, S.; Lupton, J. M.; Fernandez-Alberti, S. Excitation Energy Transfer Between Bodipy Dyes in A Symmetric Molecular Excitonic Seesaw. *Journal of Physical Chemistry A* (2021). DOI: 10.1021/Acs.Jpca.1c06332.

84. Galindo, J. F.; Freixas, V. M.; Tretiak, S.; Fernandez-Alberti, S. Back-and-Forth Energy Transfer During Electronic Relaxation in A Chlorin-Perylene Dyad. *Journal of Physical Chemistry Letters* (2021). DOI: 10.1016/J.Actamat.2021.117215.

85. Garland, A. P.; White, B. C.; Jensen, S. C.; Boyce, B. L. Pragmatic Generative Optimization of Novel Structural Lattice Metamaterials with Machine Learning. *Materials & Design* (2021). DOI: 10.1016/J.Matdes.2021.109632.

86. Gennaro, S. D.; Goldflam, M.; Burckel, D. B.; Jeong, J.; Sinclair, M. B.; Brener, I. Dielectric Metasurfaces Made from Vertically Oriented Nanoresonators. *Journal of The Optical Society of America B-Optical Physics* (2021). DOI: 10.1364/Josab.424442.

87. Ghosh, C.; Singh, M. K.; Parida, S.; Dobley, A.; Dongare, A. M.; Carter, C. B. Characterizing Li in Partially Lithiated Layer Materials Using Atomic-Resolution Imaging, Modeling, and Simulation. *Journal of The American Ceramic Society* (2021). DOI: 10.1111/Jace.18189.

88. Ghosh, C.; Singh, M. K.; Parida, S.; Janish, M. T.; Dobley, A.; Dongare, A. M.; Carter, C. B. P. Phase Evolution and Structural Modulation During in-Situ Lithiation of Mos_2, Ws_2 and Graphite in Tem. *Scientific Reports* (2021). DOI: 10.1038/S41598-021-88395-1.

89. Ghosh, D.; Ivanov, S. A.; Tretiak, S. Structural Dynamics and Electronic Properties of Semiconductor Quantum Dots: Computational Insights. *Chemistry of Materials* (2021). DOI: 10.3390/Nano11102538.

90. Giannini, N.; Yang, Z.; Rai, A. K.; Albrecht, A. R.; Sheik-Bahae, M. Near-Unity External Quantum Efficiency in Gaas/Algaas Heterostructures Grown by Molecular Beam Epitaxy. *Physica Status Solidi-Rapid Research Letters* (2021). DOI: 10.1002/Pssr.202100106.

91. Gokcan, H.; Isayev, O. Learning Molecular Potentials with Neural Networks. *Wiley Interdisciplinary Reviews-Computational Molecular Science* (2021). DOI: 10.1002/Wcms.1564.

92. Gomez, D. T.; Pratt, L. R.; Rogers, D. M.; Rempe, S. B. Free Energies of Hydrated Halide Anions: High Through-Put Computations on Clusters to Treat Rough Energy-Landscapes. *Molecules* (2021). DOI: 10.3390/Molecules26113087.

93. Goriparti, S.; Harrison, K. L.; Jungjohann, K. L. Degradation-Resistant Tio_2@Sn Anodes for High-Capacity Lithium-Ion Batteries. *Journal of Materials Science* (2021). DOI: 10.1007/S10853-021-06265-7.

94. Goriparti, S.; Mcgrath, A. J.; Rosenberg, S. G.; Siegal, M. P.; Ivanov, S. A.; Harrison, K. L. $Mnsn_2$ and $Mnsn_2$-Tio_2 Nanostructured Anode Materials for Lithium-Ion Batteries. *Nanotechnology* (2021). DOI: 10.1088/1361-6528/Ac07cf.

95. Granberg, F.; Wang, X.; Chen, D.; Jin, K.; Wang, Y.; Bei, H.; Weber, W. J.; Zhang, Y.; More, K. L.; Nordlund, K.; Djurabekova, F. Origin of Increased Helium Density Inside Bubbles in $Ni_{(1-X)}Fe_x$ Alloys. *Scripta Materialia* (2021). DOI: 10.1016/J.Scriptamat.2020.08.051.

96. Griesbach, C.; Jeon, S.-J.; Rojas, D. F.; Ponga, M.; Yazdi, S.; Pathak, S.; Mara, N.; Thomas, E. L.; Thevamaran, R. Origins of Size Effects in Initially Dislocation-Free Single-Crystal Silver Micro- and Nanocubes. *Acta Materialia* (2021). DOI: 10.1016/J.Actamat.2021.117020.

97. Canning, G. A.; Azzam, S. A.; Hoffman, A. S.; Boubnov, A.; Alshafei, F. H.; Ghosh, R.; Ko, B.; Datye, A.; Bare, S. R.; Simonetti, D. A. Lanthanum Induced Lattice Strain Improves Hydrogen Sulfide Capacities of Copper Oxide Adsorbents. *Aiche Journal* (2021). DOI: 10.1002/Aic.17484.

98. Gu, Y.; Serna, M., I; Mohan, S.; Londono-Calderon, A.; Ahmed, T.; Huang, Y.; Lee, J.; Walia, S.; Pettes, M. T.; Liechti, K. M.; Akinwande, D. Sulfurization Engineering of One-Step Low-Temperature Mos_2 and Ws_2 Thin Films for Memristor Device Applications. *Advanced Electronic Materials* (2021). DOI: 10.1002/Aelm.202100515.

99. Gutierrez-Meza, E.; Malatesta, R.; Li, H.; Bargigia, I.; Kandada, A. R. S.; Valverde-Chavez, D. A.; Kim, S.-M.; Li, H.; Stingelin, N.; Tretiak, S.; Bittner, E. R.; Silva-Acuna, C. Frenkel Biexcitons in Hybrid Hj Photophysical Aggregates. *Science Advances* (2021). DOI: 10.1126/Sciadv.Abi5197.

100. Guziewski, M.; De Oca Zapiain, D. M.; Dingreville, R.; Coleman, S. P. Microscopic and Macroscopic Characterization of Grain Boundary Energy and Strength in Silicon Carbide Via Machine-Learning Techniques. *Acs Applied Materials & Interfaces* (2021). DOI: 10.1021/Acsami.0c15980.

101. Haberkorn, N.; Zhang, Y. Y.; Bi, Z. X.; Park, B. H.; Civale, L.; Jia, Q. X. Effect of Co_2n Impurity on the Superconducting Properties of Delta-Mon Thin Films Grown by Polymer Assisted Deposition. *Materials Chemistry and Physics* (2021). DOI: 10.1016/J.Matchemphys.2020.124184.

102. Hackett, L.; Miller, M.; Brimigion, F.; Dominguez, D.; Peake, G.; Tauke-Pedretti, A.; Arterburn, S.; Friedmann, T. A.; Eichenfield, M. Towards Single-Chip Radiofrequency Signal Processing Via Acoustoelectric Electron-Phonon Interactions. *Nature Communications* (2021). DOI: 10.1038/S41467-021-22935-1.

103. Xiong, H.; Kunwar, D.; Jiang, D.; García-Vargas, C. E.; Li, H.; Du, C.; Canning, G.; Pereira-Hernandez, X. I.; Wan, Q.; Lin, S.; Purdy, S. C.; Miller, J. T.; Leung, K.; Chou, S. S.; Brongersma, H. H.; Ter Veen, R.; Huang, J.; Guo, H.; Wang, Y.; Datye, A. K. Engineering Catalyst Supports to Stabilize Pdo_x Two-Dimensional Rafts for Water-Tolerant Methane Oxidation. *Nature Catalysis* (2021). DOI: 10.1038/S41929-021-00680-4.

104. Halaby, S.; Martynowycz, M. W.; Zhu, Z.; Tretiak, S.; Zhugayevych, A.; Gonen, T.; Seifrid, M. Microcrystal Electron Diffraction for Molecular Design of Functional Non-Fullerene Acceptor Structures. *Chemistry of Materials* (2021). DOI: 10.1021/Acs.Chemmater.0c04111.

105. Hale, L. L.; Harris, C. T.; Luk, T. S.; Addamane, S. J.; Reno, J. L.; Brener, I.; Mitrofanov, O. Highly Efficient Terahertz Photoconductive Metasurface Detectors Operating at Microwatt-Level Gate Powers. *Optics Letters* (2021). DOI: 10.1364/Ol.427798.

106. Hamann, D. M.; Rudin, S. P.; Asaba, T.; Ronning, F.; Cordova, D. L. M.; Lu, P.; Johnson, D. C. Predicting and Synthesizing Interface Stabilized 2d Layers. *Chemistry of Materials* (2021). DOI: 10.1021/Acs.Chemmater.1c01064.

107. Han, J.; Wartenberg, M. G.; Chan, H. L.; Derby, B. K.; Li, N.; Scully, J. R. Electrochemical Stability, Physical, and Electronic Properties of Thermally Pre-Formed Oxide Compared to Artificially Sputtered Oxide on Fe Thin Films in Aqueous Chloride. *Corrosion Science* (2021). DOI: 10.1016/J.Corsci.2021.109456.

108. Han, Y.; Iduoku, K.; Grant, G.; Rasulev, B.; Leontyev, A.; Hobbie, E. K.; Tretiak, S.; Kilina, S., V; Kilin, D. S. Hot Carrier Dynamics at Ligated Silicon (111) Surfaces: A Computational Study.

Journal of Physical Chemistry Letters (2021). DOI: 10.1021/Acs.Jpclett.1c02084.

109. Harris, C. T.; Lu, T.-M. A Ptnige Resistance Thermometer for Cryogenic Applications. *Review of Scientific Instruments* (2021). DOI: 10.1063/5.0014007.

110. Harrison, K. L.; Goriparti, S.; Merrill, L. C.; Long, D. M.; Warren, B.; Roberts, S. A.; Perdue, B. R.; Casias, Z.; Cuillier, P.; Boyce, B. L.; Jungjohann, K. L. Effects of Applied Interfacial Pressure on Li-Metal Cycling Performance and Morphology in 4 M Lifsi in Dme. *Acs Applied Materials & Interfaces* (2021). DOI: 10.1021/Acsami.1c06488.

111. Harrison, K. L.; Merrill, L. C.; Long, D. M.; Randolph, S. J.; Goriparti, S.; Christian, J.; Warren, B.; Roberts, S. A.; Harris, S. J.; Perry, D. L.; Jungjohann, K. L. Cryogenic Electron Microscopy Reveals That Applied Pressure Promotes Short Circuits in Li Batteries. *Iscience* (2021). DOI: 10.1016/J.Isci.2021.103394.

112. Hartsfield, T. M.; Lang, J. M., Jr.; Goodwin, P. M.; Veeser, L. R. A Comparison of Raman and Pyrometry Dynamic Temperature Measurements of Shocked Cyclohexane. *Journal of Applied Physics* (2021). DOI: 10.1063/5.0039288.

113. Harvey, C.; El Atwani, O.; Kim, H.; Lavender, C.; Mccoy, M.; Sornin, D.; Lewandowski, J.; Maloy, S. A.; Pathak, S. Microstructural and Micro-Mechanical Analysis of 14ywt Nanostructured Ferritic Alloy After Varying Thermo-Mechanical Processing Paths into Tubing. *Materials Characterization* (2021). DOI: 10.1016/J.Matchar.2020.110744.

114. Harvey, C.; Torrez, A. J.; Lam, S.; Kim, H.; Maloy, S. A.; Gigax, J. G. Demonstration of A High-Throughput Tensile Testing Technique Using Femtosecond Laser-Fabricated Tensile Bars in Aisi 316 and Additively Manufactured Grade 91 Steel. *Jom* (2021). DOI: 10.1021/Acs.Nanolett.1c01670.

115. Haseman, M.; Somodi, C. B.; Stepanov, P.; Wall, D. E.; Boatner, L. A.; Hosemann, P.; Wang, Y. Q.; Uberuaga, B. P.; Selim, F. A. Neutron Irradiation Induced Defects in Oxides and Their Impact on the Oxide Properties. *Journal of Applied Physics* (2021). DOI: 10.1063/5.0046292.

116. Hattar, K.; Jungjohann, K. L. Possibility of An Integrated Transmission Electron Microscope: Enabling Complex in-Situ Experiments. *Journal of Materials Science* (2021). DOI: 10.1007/S10853-020-05598-Z.

117. He, M.; Lindsay, L.; Beechem, T. E.; Folland, T.; Matson, J.; Watanabe, K.; Zavalin, A.; Ueda, A.; Collins, W. E.; Taniguchi, T.; Caldwell, J. D. Phonon Engineering of Boron Nitride Via Isotopic Enrichment. *Journal of Materials Research* (2021). DOI: 10.1364/Ome.427591.

118. He, Y.; Jiang, L.; Chen, T.; Xu, Y.; Jia, H.; Yi, R.; Xue, D.; Song, M.; Genc, A.; Bouchet-Marquis, C.; Pullan, L.; Tessner, T.; Yoo, J.; Li, X.; Zhang, J.-G.; Zhang, S.; Wang, C. Progressive Growth of The Solid-Electrolyte Interphase Towards The Si Anode Interior Causes Capacity Fading. *Nature Nanotechnology* (2021). DOI: 10.1038/S41565-021-00947-8.

119. Hernandez, J. A.; Fonseca, L. F.; Pettes, M. T.; Jose-Yacaman, M. Thermoelectric Properties of Antimony Selenide Hexagonal Nanotubes. *Nanotechnology* (2021). DOI: 10.1088/1361-6528/Abcb31.

120. Hettiarachchi, E.; Ivanov, S.; Kieft, T.; Goldstein, H. L.; Moskowitz, B. M.; Reynolds, R. L.;

Rubasinghege, G. Atmospheric Processing of Iron-Bearing Mineral Dust Aerosol and Its Effect On Growth of A Marine Diatom, Cyclotella Meneghiniana. *Environmental Science & Technology* (2021). DOI: 10.1021/Acs.Est.0c06995.

121. Huang, H.-H.; Tsai, H.; Raja, R.; Lin, S.-L.; Ghosh, D.; Hou, C.-H.; Shyue, J.-J.; Tretiak, S.; Chen, W.; Lin, K.-F.; Nie, W.; Wang, L. Robust Un-Encapsulated Perovskite Solar Cells Protected by A Fluorinated Fullerene Electron Transporting Layer. *Acs Energy Letters* (2021). DOI: 10.1021/Acsenergylett.1c01526.

122. Hu, C.; Dernov, A.; Xu, H.; Drozdov, G.; Dumitrica, T. Ab Initio Predictions of Graphite-Like Phase with Anomalous Grain Boundaries and Flexoelectricity from Collapsed Carbon Nanotubes. *Journal of Chemical Physics* (2021). DOI: 10.1063/5.0038666.

123. Hu, C.; Medlin, D. L.; Dingreville, R. Disconnection-Mediated Transition in Segregation Structures at Twin Boundaries. *Journal of Physical Chemistry Letters* (2021). DOI: 10.1021/Acs.Jpclett.1c02189.

124. Zhao, H.; Pettes, M. T.; Zheng, Y.; Htoon, H. Site-Controlled Telecom-Wavelength Single-Photon Emitters in Atomically-Thin Mote2. *Nature Communications* (2021). DOI: 10.1038/S41467-021-27033-W.

125. Huang, H.-H.; Liu, Q.-H.; Tsai, H.; Shrestha, S.; Su, L.-Y.; Chen, P.-T.; Chen, Y.-T.; Yang, T.-A.; Lu, H.; Chuang, C.-H.; Lin, K.-F.; Rwei, S.-P.; Nie, W.; Wang, L. A Simple One-Step Method with Wide Processing Window for High-Quality Perovskite Mini-Module Fabrication. *Joule* (2021). DOI: 10.1016/J.Joule.2021.02.012.

126. Huang, J.; Phuah, X. L.; Mcclintock, L. M.; Padmanabhan, P.; Vikrant, K. S. N.; Wang, H.; Zhang, D.; Wang, H.; Lu, P.; Gao, X.; Sun, X.; Xu, X.; Garcia, R. E.; Chen, H.-T.; Zhang, X.; Wang, H. Core-Shell Metallic Alloy Nanopillars-in-Dielectric Hybrid Metamaterials with Magneto-Plasmonic Coupling. *Materials Today* (2021). DOI: 10.1016/J.Mattod.2021.10.024.

127. Kim, H.; Gigax, J. G.; El-Atwani, O.; Chancey, M. R.; Baldwin, J. K.; Wang, Y.; Maloy, S. A. Comparison of Void Swelling of Ferritic-Martensitic and Ferritic Ht9 Alloys After High-Dose Self-Ion Irradiation. *Materials Characterization* (2021). DOI: 10.1016/J.Matchar.2021.110908.

128. Imam, Z. I.; Bachand, G. D. Fabricating Multi-Component Lipid Nanotube Networks Using The Gliding Kinesin Motility Assay. *Jove-Journal of Visualized Experiments* (2021). DOI: 10.3791/60899.

129. Innes-Gold, S. N.; Jacobson, D. R.; Pincus, P. A.; Stevens, M. J.; Saleh, O. A. Flexible, Charged Biopolymers in Monovalent and Mixed-Valence Salt: Regimes of Anomalous Electrostatic Stiffening and of Salt Insensitivity. *Physical Review E* (2021). DOI: 10.1103/Physreve.104.014504.

130. Islam, Z.; Barr, C. M.; Hattar, K.; Haque, A. Defect Annihilation in Heavy Ion Irradiated Polycrystalline Gold. *Materials Letters* (2021). DOI: 10.1016/J.Matlet.2020.128694.

131. Ivie, J. A.; Campbell, Q.; Koepke, J. C.; Brickson, M., I; Schultz, P. A.; Muller, R. P.; Mounce, A. M.; Ward, D. R.; Carroll, M. S.; Bussmann, E.; Baczewski, A. D.; Misra, S. Impact of Incorporation Kinetics on Device Fabrication with Atomic Precision. *Physical Review Applied*

(2021). DOI: 10.1103/Physrevapplied.16.054037.

132. Jabed, M. A.; Zhao, J.; Kilin, D.; Yu, T. Understanding of Light Absorption Properties of the N-Doped Graphene Oxide Quantum Dot with Td-Dft. *Journal of Physical Chemistry C* (2021). DOI: 10.1021/Acs.Jpcc.1c03012.

133. Jawaharram, G. S.; Barr, C. M.; Hattar, K.; Dillon, S. J. Evidence for A High Temperature Whisker Growth Mechanism Active in Tungsten During In-Situ Nanopillar Compression. *Nanomaterials* (2021). DOI: 10.3390/Nano11092429.

134. Jing, Z.; Rackers, J. A.; Pratt, L. R.; Liu, C.; Rempe, S. B.; Ren, P. Thermodynamics of Ion Binding and Occupancy in Potassium Channels. *Chemical Science* (2021). DOI: 10.1039/D1sc01887f.

135. Jonathan A. Bollinger, G. S. G., Mark J. Stevens, and Michael Rubinstein. Overlap Concentration in Salt-Free Polyelectrolyte Solutions. *Macromolecules* (2021). DOI: 10.1021/Acs.Macromol.1c01491.

136. Jones, M. R.; Delrio, F. W.; Beechem, T. E.; McDonald, A. E.; Babuska, T. F.; Dugger, M. T.; Chandross, M.; Argibay, N.; Curry, J. F. Stress- and Time-Dependent Formation of Self-Lubricating in-Situ Carbon (Slic) Films on Catalytically-Active Noble Alloys. *Jom* (2021). DOI: 10.1007/S11837-021-04809-5.

137. Jones, M. R.; Delrio, F. W.; Pegues, J. W.; Lu, P.; Puckett, R.; Bobbitt, N. S.; Hardin, T. J.; Chandross, M.; Kustas, A. B.; Argibay, N. Additive Manufacturing of High-Strength Multiphase Nanostructures in The Binary Ni-Nb System for The Discovery of New Types of Superalloys. *Journal of Materials Research* (2021). DOI: 10.1557/S43578-021-00290-7.

138. Jones, T.; Peters, W. K.; Efimov, A.; Yarotski, D.; Trebino, R.; Bowlan, P. Measuring an Ultrashort, Ultraviolet Pulse in A Slowly Responding, Absorbing Medium. *Optics Express* (2021). DOI: 10.1364/Oe.417293.

139. Choi, J.; Jin, D. K.; Jeong, J.; Kang, B. K.; Yang, W. S.; Ali, A.; Yoo, J.; Kim, M. J.; Yi, G.-C.; Hong, Y. J. Facet-Selective Morphology-Controlled Remote Epitaxy of Zno Microcrystals Via Wet Chemical Synthesis. *Scientific Reports* (2021). DOI: 10.1038/S41598-021-02222-1.

140. Jungjohann, K. L.; Gannon, R. N.; Goriparti, S.; Randolph, S. J.; Merrill, L. C.; Johnson, D. C.; Zavadil, K. R.; Harris, S. J.; Harrison, K. L. Cryogenic Laser Ablation Reveals Short-Circuit Mechanism in Lithium Metal Batteries. *Acs Energy Letters* (2021). DOI: 10.1021/Acsenergylett.1c00509.

141. Kabir, F.; Hosen, M. M.; Ding, X.; Lane, C.; Dhakal, G.; Liu, Y.; Dimitri, K.; Sims, C.; Regmi, S.; Sakhya, A. P.; Persaud, L.; Beetar, J. E.; Liu, Y.; Chini, M.; Pathak, A. K.; Zhu, J.-X.; Gofryk, K.; Neupane, M. Effect of Dilute Magnetism in A Topological Insulator. *Frontiers in Materials* (2021).DOI:10.3389/Fmats.2021.706658.

142. Kalb, D.; Vo, H. D.; Adikari, S.; Hong-Geller, E.; Munsky, B.; Werner, J. Visualization and Modeling of Inhibition of Il-1β and Tnf-A Mrna Transcription at The Single-Cell Level. *Scientific Reports* (2021). DOI: 10.1038/S41598-021-92846-0.

143. Kang, J. G.; Jang, H.; Ma, J.; Yang, Q.; Hattar, K.; Diao, Z.; Yuan, R.; Zuo, J.; Sinha, S.; Cahill, D.G.;

Braun, P., V. Ultralow Thermal Conductivity in Nanoporous Crystalline Fe_3o_4. *Journal of Physical Chemistry C* (2021). DOI: 10.1021/Acs.Jpcc.1c00411.

144. Katzenmeyer, A. M.; Dmitrovic, S.; Baczewski, A. D.; Campbell, Q.; Bussmann, E.; Lu, T.-M.; Anderson, E. M.; Schmucker, S. W.; Ivie, J. A.; Campbell, D. M.; Ward, D. R.; Scrymgeour, D. A.; Wang, G. T.; Misra, S. Photothermal Alternative to Device Fabrication Using Atomic Precision Advanced Manufacturing Techniques. *Journal of Micro-Nanopatterning Materials and Metrology-Jm3* (2021). DOI: 10.1117/1.Jmm.20.1.014901.

145. Kehayias, P.; Henshaw, J.; Ziabari, M. S.; Titze, M.; Bielejec, E.; Lilly, M. P.; Mounce, A. M. A Fitting Algorithm for Optimizing Ion Implantation Energies and Fluences. *Nuclear Instruments & Methods in Physics Research Section B-Beam Interactions with Materials and Atoms* (2021). DOI: 10.1016/J.Nimb.2021.05.014.

146. Keiser, G. R.; Karl, N.; Ul Haque, S. R.; Brener, I.; Mittleman, D. M.; Averitt, R. D. Structural Tuning of Nonlinear Terahertz Metamaterials Using Broadside Coupled Split Ring Resonators. *Aip Advances* (2021). DOI: 10.1063/5.0053876.

147. Kendall, L.; Chamaani, A.; Piontkowski, Z.; Beechem, T. E.; Ridley, M.; Opila, E. J.; Zangari, G.; Mcdonnell, S. J. Influence of Oxygen Dopants on The Her Catalytic Activity of Electrodeposited Mooxsy Electrocatalysts. *Acs Applied Energy Materials* (2021). DOI: 10.1021/Acsaem.1c02234.

148. Kim, Y.; Hu, Z.; Avdeev, I. D.; Singh, A.; Singh, A.; Chandrasekaran, V.; Nestoklon, M. O.; Goupalov, S. V.; Hollingsworth, J. A.; Htoon, H. Interplay of Bright Triplet and Dark Excitons Revealed by Magneto-Photoluminescence of Individual Pbs/Cds Quantum Dots. *Small* (2021). DOI:10.1002/Smll.202006977.

149. Kim, Y.; Kim, D.; Auchter, E.; Marquez, J.; Tutchton, R.; Li, N.; Luk, T. S.; Dervishi, E.; Kim, Y.-J.; Zhu, J.-X.; Yoo, J. Recyclable Graphene Sheets as a Growth Template for Crystalline Zno Nanowires. *Nanomaterials* (2021). DOI: 10.3390/Nano11082093.

150. Kobbekaduwa, K.; Shrestha, S.; Adhikari, P.; Liu, E.; Coleman, L.; Zhang, J.; Shi, Y.; Zhou, Y.; Bekenstein, Y.; Yan, F.; Rao, A. M.; Tsai, H.; Beard, M. C.; Nie, W.; Gao, J. in-Situ Observation of Trapped Carriers in Organic Metal Halide Perovskite Films with Ultra-Fast Temporal and Ultra-High Energetic Resolutions. *Nature Communications* (2021). DOI: 10.1038/S41467-021-21946-2.

151. Kort-Kamp, W. J. M.; Azad, A. K.; Dalvit, D. A. R. Space-Time Quantum Metasurfaces. *Physical Review Letters* (2021). DOI: 10.1103/Physrevlett.127.043603.

152. Koski, J. P.; Frischknecht, A. L. Self-Assembled Vesicles from Mixed Brush Nanoparticles in Solution.*Macromolecules* (2021). DOI: 10.1021/Acs.Macromol.1c00503.

153. Krishnamurthy, S.; Singh, A.; Hu, Z.; Blake, A., V; Kim, Y.; Singh, A.; Dolgopolova, E. A.; Williams, D. J.; Piryatinski, A.; Malko, A., V; Htoon, H.; Sykora, M.; Hollingsworth, J. A. Pbs/Cds Quantum Dot Room-Temperature Single-Emitter Spectroscopy Reaches The Telecom O and S Bands Via An Engineered Stability. *Acs Nano* (2021). DOI: 10.1021/Acsnano.0c05907.

154. Kriso, C.; Bergmeier, T.; Giannini, N.; Albrecht, A. R.; Sheik-Bahae, M.; Benis, S.; Faryadras, S.;

Van Stryland, E. W.; Hagan, D. J.; Koch, M.; Mette, G.; Rahimi-Iman, A. Probing The Ultrafast Gain and Refractive Index Dynamics of a Vecsel. *Applied Physics Letters* (2021). DOI: Arxiv.Org/Pdf/2106.13664.Pdf.

155. Kulichenko, M.; Smith, J. S.; Nebgen, B.; Li, Y. W.; Fedik, N.; Boldyrev, A., I; Lubbers, N.; Barros, K.; Tretiak, S. The Rise of Neural Networks for Materials and Chemical Dynamics. *Journal of Physical Chemistry Letters* (2021). DOI: 10.1021/Acs.Jpclett.1c01357.

156. Kumbhakar, P.; Shanmugam, A.; Sharma, C. H.; Reno, J. L.; Thalakulam, M. Quantum Point Contact Galvanically Coupled to Planar Superconducting Resonator: A Shot-Noise-Limited Broad-Band Electrical Amplifier. *Quantum Science and Technology* (2021). DOI: 10.1088/2058-9565/Ac107f.

157. Kunka, C.; Shanker, A.; Chen, E. Y.; Kalidindi, S. R.; Dingreville, R. Decoding Defect Statistics from Diffractograms Via Machine Learning. *Npj Computational Materials* (2021). DOI: 10.1038/S41524-021-00539-Z.

158. Lang, E.; Dennett, C. A.; N. Madden, N.; Hattar, K. The in-Situ Ion Irradiation Toolbox: Time-Resolved Structure and Property Measurements. *Jom* (2021). DOI: DOI.Org/10.1007/S11837-021-04993-4.

159. Langer, M.; Paloncyova, M.; Medved, M.; Pykal, M.; Nachtigallova, D.; Shi, B.; Aquino, A. J. A.; Lischka, H.; Otyepka, M. Progress and Challenges in Understanding of Photoluminescence Properties of Carbon Dots Based On Theoretical Computations. *Applied Materials Today* (2021). DOI: 10.1016/J.Apmt.2020.100924.

160. El Khoury, L.; Mobley, D. Ye, D.; Rempe, S. Enhancing Paraoxon Binding to Organophosphorus Hydrolase Active Site. *International Journal of Molecular Sciences* (2021). DOI: 10.26434/Chemrxiv.13930874.V1.

161. Lee, H.; Shabani, M.; Pataky, G. J.; Abdeljawad, F. Tensile Deformation Behavior of Twist Grain Boundaries in High Entropy Alloy Bicrystals. *Scientific Reports* (2021). DOI: 10.1038/S41598-020-77487-Z.

162. Pan, L.; Shrestha, S.; Taylor, N.; Nie, W.; Cao, L. R. Determination of X-Ray Detection Limit and Applications in Perovskite X-Ray Detectors. *Nature Communications* (2021). DOI: 10.1038/S41467-021-25648-7.

163. Vidmar, L.; Krajewski, B.; Bonča, J.; Mierzejewski, M. Phenomenology of Spectral Functions in Disordered Spin Chains at Infinite Temperature. *Physical Review Letters* (2021). DOI: 10.1103/Physrevlett.127.230603.

164. Leverant, C.; Priest, C.; Greathouse, J.; Rempe, S.; Barton, P.; Kinnan, A. M. Quantum Calculations of Vx Ammonolysis and Hydrolysis Pathways Via Hydrated Lithium Nitride. *International Journal of Molecular Sciences* (2021). DOI: 10.3390/Ijms22168653.

165. Lewis, S. G.; Ghosh, D.; Jensen, K. L.; Finkenstadt, D.; Shabaev, A.; Lambrakos, S. G.; Liu, F.; Nie, W.; Blancon, J.-C.; Zhou, L.; Crochet, J. J.; Moody, N.; Mohite, A. D.; Tretiak, S.; Neukirch, A. J. Cesium-Coated Halide Perovskites As A Photocathode Material: Modeling Insights. *Journal of Physical Chemistry Letters* (2021). DOI: 10.1021/Acs.Jpclett.1c01412.

166. Li, M. M.; Ivanov, S. A. The Intrinsic Electrochemical Behavior of Layered Nanoparticles. *Nanotechnology* (2022). DOI: 10.1088/1361-6528/Ac4132.

167. Li, Q.; Shang, Z.; Sun, X.; Fan, C.; Su, R.; Richter, N. A.; Fan, Z.; Zhang, Y.; Xue, S.; Wang, H.; Zhang, X. High-Strength and Tunable Plasticity in Sputtered Al-Cr Alloys with Multistage Phase Transformations. *International Journal of Plasticity* (2021). DOI: 10.1016/J.Ijplas.2020.102915.

168. Li, Q.; Wang, J.; Wang, H.; Zhang, X. Achieving Strong and Stable Nanocrystalline Al Alloys Through Compositional Design. *Journal of Materials Research* (2021). DOI: 10.1557/S43578-021-00363-7.

169. Li, W.; Taylor, M. G.; Bayerl, D.; Mozaffari, S.; Dixit, M.; Ivanov, S.; Seifert, S.; Lee, B.; Shanaiah, N.; Lu, Y.; Kovarik, L.; Mpourmpakis, G.; Karim, A. M. Solvent Manipulation of The Pre-Reduction Metal-Ligand Complex and Particle-Ligand Binding for Controlled Synthesis of Pd Nanoparticles. *Nanoscale* (2021). DOI: 10.1039/D0nr06078j.

170. Lin, E. Y.; Frischknecht, A. L.; Riggleman, R. A. Chain and Segmental Dynamics in Polymer-Nanoparticle Composites with High Nanoparticle Loading. *Macromolecules* (2021). DOI: 10.1021/Acs.Macromol.1c00206.

171. Lin, E. Y.; Frischknecht, A. L.; Winey, K. I.; Riggleman, R. A. Effect of Surface Properties and Polymer Chain Length on Polymer Adsorption in Solution. *Journal of Chemical Physics* (2021). DOI: 10.1063/5.0052121.

172. Lingappa, U. F., Yeager, C.M., Sharma, A., Lanza, N.L., Morales, D.P., Xie, G., Atencio, A.D., Chadwick, G.L., Monteverde, D.R., Magyar, J.S. and Webb, S.M. An Ecophysiological Explanation for Manganese Enrichment in Rock Varnish. *Proceedings of The National Academy of Sciences* (2021). DOI: 10.1073/Pnas.2025188118.

173. Lionello, D. F.; Ramallo, J., I; Caro, M.; Wang, Y. Q.; Sheehan, C.; Baldwin, J. K.; Nogan, J.; Caro, A.; Fuertes, M. C.; Ruestes, C. J. Mechanical Properties of Al2o3-Functionalized Nanoporous Gold Foams Under Irradiation. *Journal of Materials Research* (2021). DOI: 10.1557/S43578-021-00262-X.

174. Liu, F.; Guo, L.; Defazio, J.; Pavlenko, V.; Yamamoto, M.; Moody, N. A.; Yamaguchi, H. Photoemission from Bialkali Photocathodes Through an Atomically Thin Protection Layer. *Acs Applied Materials & Interfaces* (2021). DOI: 10.1021/Acsami.1c19393.

175. Liu, F.; Sidhik, S.; Hoffbauer, M. A.; Lewis, S.; Neukirch, A. J.; Pavlenko, V.; Tsai, H.; Nie, W.; Even, J.; Tretiak, S.; Ajayan, P. M.; Kanatzidis, M. G.; Crochet, J. J.; Moody, N. A.; Blancon, J.-C.; Mohite, A. D. Highly Efficient Photoelectric Effect in Halide Perovskites for Regenerative Electron Sources. *Nature Communications* (2021). DOI: 10.1038/S41467-021-20954-6.

176. Liu, H.; Liang, J.; Watt, J.; Tilley, R. D.; Amal, R.; Wang, D.-W. Wafer-Scale Quasi-Layered Tungstate-Doped Polypyrrole Film with High Volumetric Capacitance. *Nano Research* (2021). DOI:10.1007/S12274-021-3783-3.

177. Liu, P.; Hao, H.; Celio, H.; Cui, J.; Ren, M.; Wang, Y.; Dong, H.; Chowdhury, A. R.; Hutter, T.; Perras, F. A.; Nanda, J.; Watt, J.; Mitlin, D. Multifunctional Separator Allows Stable Cycling of

Potassium Metal Anodes and of Potassium Metal Batteries. *Advanced Materials* (2021). DOI: 10.1002/Adma.202105855.

178. Liu, Y.; Vasudevan, R. K.; Kelley, K. K.; Kim, D.; Sharma, Y.; Ahmadi, M.; Kalinin, S., V; Ziatdinov, M. Decoding the Shift-Invariant Data: Applications for Band-Excitation Scanning Probe Microscopy. *Machine Learning-Science and Technology* (2021). DOI: Https://Arxiv.Org/Ftp/Arxiv/Papers/2104/2104.10207.Pdf.

179. Londono-Calderon, A.; Williams, D. J.; Schneider, M.; Savitzky, B. H.; Ophus, C.; Pettes, M. T. Local Lattice Deformation of Tellurene Grain Boundaries by Four-Dimensional Electron Microscopy. *Journal of Physical Chemistry C* (2021). DOI: 10.1021/Acs.Jpcc.1c00308.

180. Londono-Calderon, A.; Williams, D. J.; Schneider, M. M.; Savitzky, B. H.; Ophus, C.; Ma, S.; Zhu, H.; Pettes, M. T. Intrinsic Helical Twist and Chirality in Ultrathin Tellurium Nanowires. *Nanoscale* (2021). DOI:10.1039/D1nr01442k.

181. Long, S.; Cai, S.; Schonemann, R.; Rosa, P. F. S.; Balicas, L.; Huang, C.; Guo, J.; Zhou, Y.; Han, J.; Zhou, L.; Li, Y.; Li, X.; Wu, Q.; Weng, H.; Xiang, T.; Sun, L. Observation of Nearly Identical Superconducting Transition Temperatures in The Pressurized Weyl Semimetals *M* $Irte_4$ (M = Nb and Ta). *Physical Review B* (2021). DOI: 10.1103/Physrevb.104.144503.

182. Lu, L.; Pan, Q.; Hattar, K.; Boyce, B. L. Fatigue and Fracture of Nanostructured Metals and Alloys. *Mrs Bulletin* (2021). DOI: 10.1557/S43577-021-00054-Y.

183. Daly, L.; Lee, M. R.; Hallis, L. J.; Ishii, H. A.; Bradley, J. P.; Bland, P. A.; Saxey, D. W.; Fougerouse, D.; Rickard, W. D.; Forman, L. V.; Timms, N. E.; Jourdan, F.; Reddy, S. M.; Salge, T.; Quadir, Z.; Christou, E.; Cox, M. A.; Aguiar, J. A.; Hattar, K.; Monterrosa, A.; Keller, L. P.; Christoffersen, R.; Dukes, C. A.; Loeffler, M. J.; Thompson, M. S. Solar Wind Contributions to Earth's Oceans. *Nature Astronomy* (2021). DOI:10.1038/S41550-021-01487-W.

184. Lydzba, P.; Bonca, J. Long-Lived Nonthermal States in Pumped One-Dimensional Systems of Hard-Core Bosons. *Physical Review B* (2021). DOI: 10.1103/Physrevb.103.184310.

185. Lystrom, L.; Roberts, A.; Dandu, N.; Kilina, S. Surface-Induced Deprotonation of Thiol Ligands Impacts the Optical Response of Cds Quantum Dots. *Chemistry of Materials* (2021). DOI: 10.1021/Acs.Chemmater.0c03610.

186. Magedov, S.; Koh, C.; Malone, W.; Lubbers, N.; Nebgen, B. Bond Order Predictions Using Deep Neural Networks. *Journal of Applied Physics* (2021). DOI: 10.1063/5.0016011.

187. Matthews, B. E.; Sassi, M.; Barr, C.; Ophus, C.; Kaspar, T. C.; Jiang, W.; Hattar, K.; Spurgeon, S. R. Percolation of Ion-Irradiation-Induced Disorder in Complex Oxide Interfaces. *Nano Letters* (2021). DOI: 10.1021/Acs.Nanolett.1c01651.

188. Powers, M.; Stewart, J. A.; Dingreville, R.; Derby, B. K.; Misra, A. Compositionally-Driven Formation Mechanism of Hierarchical. *Nanomaterials* (2021). DOI: 10.3390/Nano11102635

189. Mccabe, R. J.; Nizolek, T. J.; Li, N.; Zhang, Y.; Coughlin, D. R.; Miller, C.; Carpenter, J. S. Evolution of Microstructures and Properties Leading to Layer Instabilities During Accumulative Roll Bonding of Fe-Cu, Fe-Ag, and Fe-Al. *Materials & Design* (2021). DOI:

10.1116/6.0001406.

190. Mia, M. B.; Ahmed, S. Z.; Jaidye, N.; Ahmed, I.; Kim, S. Mode-Evolution-Based Ultra-Broadband Polarization Beam Splitter Using Adiabatically Tapered Extreme Skin-Depth Waveguide. *Optics Letters* (2021). DOI: 10.1364/Ol.434110.

191. Meng, L.; Duwal, S.; Lane, J. M. D.; Ao, T.; Stoltzfus, B.; Knudson, M.; Park, C.; Chow, P.; Xiao, Y.; Fan, H.; Qin, Y. Pressure Induced Assembly and Coalescence of Lead Chalcogenide Nanocrystals. *Journal of The American Chemical Society* (2021). DOI: 10.1021/Jacs.0c13350.

192. Merrill, L. C.; Rosenberg, S. G.; Jungjohann, K. L.; Harrison, K. L. Uncovering the Relationship Between Aging and Cycling on Lithium Metal Battery Self-Discharge. *Acs Applied Energy Materials* (2021). DOI: 10.1021/Acsaem.1c00874.

193. Migdisov, A.; Nisbet, H.; Li, N.; White, J.; Xu, H.; Nelson, A.; Roback, R. Instability of U_3si_2 in Pressurized Water Media at Elevated Temperatures. *Communications Chemistry* (2021). DOI: 10.1038/S42004-021-00504-3.

194. Mishra, A.; Kunka, C.; Echeverria, M. J.; Dingreville, R.; Dongare, A. M. Fingerprinting Shock-Induced Deformations Via Diffraction. *Scientific Reports* (2021). DOI: 10.1038/S41598-021-88908-Y.

195. Misra, A.; Goeken, M.; Mara, N. A.; Beyerlein, I. J. Hierarchical and Heterogeneous Multiphase Metallic Nanomaterials and Laminates. *Mrs Bulletin* (2021). DOI: 10.1557/S43577-021-00059-7.

196. Moore, R. D.; Beecroft, T.; Rohrer, G. S.; Barr, C. M.; Homer, E. R.; Hattar, K.; Boyce, B. L.; Abdeljawad, F. The Grain Boundary Stiffness and Its Impact on Equilibrium Shapes and Boundary Migration: Analysis of The Sigma 5, 7, 9, and 11 Boundaries in Ni. *Acta Materialia* (2021). DOI: 10.1016/J.Apmt.2021.101187.

197. Sirica, N.; Hedayat, H.; Bugini, D.; Koehler, M. R.; Li, L.; Parker, D. S.; Mandrus, D. G.; Dallera, C.; Carpene, E.; Mannella, N. Disentangling Electronic, Lattice, and Spin Dynamics in The Chiral Helimagnet $Cr_{1/3}nbs_2$. *Physical Review B* (2021). DOI:10.1103/Physrevb.104.174426.

198. Nandakumaran, N.; Barnsley, L.; Feoktystov, A.; Ivanov, S. A.; Huber, D. L.; Fruhner, L. S.; Leffler, V.; Ehlert, S.; Kentzinger, E.; Qdemat, A.; Bhatnagar-Schoeffmann, T.; Ruecker, U.; Wharmby, M. T.; Cervellino, A.; Dunin-Borkowski, R. E.; Brueckel, T.; Feygenson, M. Unravelling Magnetic Nanochain Formation in Dispersion for in Vivo Applications. *Advanced Materials* (2021). DOI: 10.1002/Adma.202008683.

199. Narvaez Villarrubia, C. W.; Tumas, K. C.; Chauhan, R.; Macdonald, T.; Dattelbaum, A. M.; Omberg, K.; Gupta, G. Long-Term Stabilization of Dna at Room Temperature Using a One-Step Microwave Assisted Process. *Emergent Materials* (2021). DOI: 10.1007/S42247-021-00208-3.

200. Nathaniel, J. E., Ii; Vetterick, G. A.; El-Atwani, O.; Leff, A.; Baldwin, J. K.; Baldo, P.; Kirk, M. A.; Hattar, K.; Taheri, M. L. The Influence of Solute on Irradiation Damage Evolution in Nanocrystalline Thin-Films. *Journal of Nuclear Materials* (2021). DOI: 10.1016/J.Jnucmat.2020.152616.

201. Neuman, T.; Eichenfield, M.; Trusheim, M. E.; Hackett, L.; Narang, P.; Englund, D. A Phononic Interface Between A Superconducting Quantum Processor and Quantum Networked Spin Memories. *Npj Quantum Information* (2021). DOI: 10.1038/S41534-021-00457-4.

202. Nieman, R.; Aquino, A. J. A.; Lischka, H. Exploration of Graphene Defect Reactivity Toward A Hydrogen Radical Utilizing a Preactivated Circumcoronene Model. *Journal of Physical Chemistry A* (2021). DOI: 10.1021/Acs.Jpca.0c09255.

203. Owen, J. H. G.; Campbell, Q.; Santini, R.; Ivie, J. A.; Baczewski, A. D.; Schmucker, S. W.; Bussmann, E.; Misra, S.; Randall, J. N. Al-Alkyls as Acceptor Dopant Precursors for Atomic-Scale Devices. *Journal of Physics-Condensed Matter* (2021). DOI: 10.1088/1361-648x/Ac1ddf.

204. Pace, N. A.; Hennelly, S. P.; Goodwin, P. M. Immobilization of Cyanines in Dna Produces Systematic Increases in Fluorescence Intensity. *Journal of Physical Chemistry Letters* (2021). DOI: 10.1021/Acs.Jpclett.1c02022.

205. Pan, W.; Soh, D.; Yu, W.; Davids, P.; Nenoff, T. M. Microwave Response in A Topological Superconducting Quantum Interference Device. *Scientific Reports* (2021). DOI: 10.1038/S41598-021-88035-8.

206. Paren, B. A.; Thurston, B. A.; Kanthawar, A.; Neary, W. J.; Kendrick, A.; Marechal, M.; Kennemur, J. G.; Stevens, M. J.; Frischknecht, A. L.; Winey, K., I. Fluorine-Free Precise Polymer Electrolyte for Efficient Proton Transport: Experiments and Simulations. *Chemistry of Materials* (2021). DOI: 10.1021/Acs.Chemmater.1c01443.

207. Parisi, D.; Costanzo, S.; Jeong, Y.; Ahn, J.; Chang, T.; Vlassopoulos, D.; Halverson, J. D.; Kremer, K.; Ge, T.; Rubinstein, M.; Grest, G. S.; Srinin, W.; Grosberg, A. Y. Nonlinear Shear Rheology of Entangled Polymer Rings. *Macromolecules* (2021). DOI: 10.1021/Acs.Macromol.0c02839.

208. Paudel, B.; Kang, K. T.; Sharma, Y.; Nakotte, H.; Yarotski, D.; Chen, A. Symmetry Mismatch Controlled Ferroelastic Domain Ordering and The Functional Properties of Manganite Films On Cubic Miscut Substrates. *Physical Chemistry Chemical Physics* (2021). DOI: 10.1039/D1cp01957k.

209. Pavunny, S. P.; Yeats, A. L.; Banks, H. B.; Bielejec, E.; Myers-Ward, R. L.; Dejarld, M. T.; Bracker, A. S.; Gaskill, D. K.; Carter, S.G. Arrays of Si Vacancies in 4h-Sic Produced by Focused Li Ion Beam Implantation. *Scientific Reports* (2021). DOI: 10.1038/S41598-021-82832-X.

210. Percival, S. J.; Russo, S.; Priest, C.; Hill, R. C.; Ohlhausen, J. A.; Small, L. J.; Rempe, S. B.; Spoerke, E. D. Bio-Inspired Incorporation of Phenylalanine Enhances Ionic Selectivity in Layer-by-Layer Deposited Polyelectrolyte Films. *Soft Matter* (2021). DOI: 10.1039/D1sm00134e.

211. Perez, C. M.; Ghosh, D.; Prezhdo, O.; Tretiak, S.; Neukirch, A. J. Excited-State Properties of Defected Halide Perovskite Quantum Dots: Insights from Computation. *Journal of Physical Chemistry Letters* (2021). DOI: 10.1021/Acs.Jpclett.0c03317.

212. Perez, C. R. K. M., M. P.; Forrest, E. C.; Tappan, A. S.; Asheghi, M.; Goodson, K. E.; Ziade, E. O. Non-Contact Mass Density and Thermal Conductivity Measurements of Organic Thin Films Using Frequency–Domain Thermoreflectance. *Advanced Materials Interfaces* (2021). DOI: 10.1002/Admi.202101404.

213. Piontkowski, Z. T.; Runnerstrom, E. L.; Cleri, A.; Mcdonald, A.; Ihlefeld, J.; Saltonstall, C.; Maria, J.-P.; Beechem, T. E. Effects of Strain, Disorder, and Coulomb Screening on Free-Carrier Mobility in Doped Cadmium Oxide. *Journal of Applied Physics* (2021). DOI: 10.1063/5.0073345.

214. Piva, M. M.; Rahn, M. C.; Thomas, S. M.; Scott, B. L.; Pagliuso, P. G.; Thompson, J. D.; Schoop, L. M.; Ronning, F.; Rosa, P. F. S. Robust Narrow-Gap Semiconducting Behavior in Square-Net $La_3cd_2as_6$. *Chemistry of Materials* (2021). DOI: 10.1021/Acs.Chemmater.1c00797.

215. Prakash, D. J.; Chen, Y.; Debasu, M. L.; Savage, D. E.; Tangpatjaroen, C.; Deneke, C.; Malachias, A.; Alfieri, A. D.; Elleuch, O.; Lekhal, K.; Szlufarska, I.; Evans, P. G.; Cavallo, F. Reconfiguration of Amorphous Complex Oxides: A Route to A Broad Range of Assembly Phenomena, Hybrid Materials, and Novel Functionalities. *Small* DOI: 10.1002/Smll.202105424.

216. Prakash, D. J.; Dwyer, M. M.; Argudo, M. M.; Debasu, M. L.; Dibaji, H.; Lagally, M. G.; Van Der Weide, D. W.; Cavallo, F. Self-Winding Helices as Slow-Wave Structures for Sub-Millimeter Traveling-Wave Tubes. *Acs Nano* (2021). DOI: 10.1021/Acsnano.0c08296.

217. Priante, D.; Zhang, M.; Albrecht, A. R.; Bek, R.; Zimmer, M.; Nguyen, C.; Follman, D.; Cole, G. D.; Sheik-Bahae, M. Demonstration of A 20-W Membrane-External-Cavity Surface-Emitting Laser for Sodium Guide Star Applications. *Electronics Letters* (2021). DOI: 10.1049/Ell2.12008.

218. Priest, C. W.; Greathouse, J. A.; Kinnan, M. K.; Burton, P. D.; Rempe, S. B. Ab Initio and Force Field Molecular Dynamics Study of Bulk Organophosphorus and Organochlorine Liquid Structures. *Journal of Chemical Physics* (2021). DOI: 10.1063/5.0033426.

219. Protsak, I.; Gun'ko, V.; Morozov, Y.; Henderson, I. M.; Zhang, D.; Yinjun, Z.; Turov, V. Intermediates of Tris (Pentafluorophenyl) Borane and Dimethyl Carbonate Pave the Way for Deeper Organosiloxane Depolymerization Reactions. *Polymer Journal* (2021). DOI: 10.1038/S41428-020-00452-0.

220. R. Wu, D. Z., T. Maity, P. Lu, J. Yang, X.Y. Gao, S.S. Zhao, X.C. Wei, H. Zeng, A. Kursumovic, G. Tian, W.W. Li, C. Yun, Y.Q. Wang, Z.Y. Ren, Z.Y. Zhou, M. Liu, K. H. L. Zhang, Q.X. Jia, J.B. Yang, H.Y. Wang and J. L. Macmanus-Driscoll. Self-Biased Magnetoelectric Switching at Room Temperature in Three-Phase Ferroelectric–Antiferromagnetic–Ferrimagnetic Nanocomposites. *Nature Electronics* (2021). DOI:10.1038/S41928-021-00584-Y.

221. Parrish, R. J.; Bufford, D. C.; Frazer, D. M.; Taylor, C. A.; Gutierrez-Kolar, J.; Buller, D. L.; Boyce, B. L.; Hattar, K. Exploring Coupled Extreme Environments Via in-Situ Transmission Electron Microscopy. *Microscopy Today* (2021). DOI: 10.1017/S1551929520001595.

222. Radhakrishnan, M., Nizolek, T., Li, N., Wang, Y., Bachhav, M., Kombaiah, B., & Anderoglu, O. Radiation-Induced Mixing and Demixing Behavior in Metallic Multilayers Exhibiting Limited Solid Miscibility. *Microscopy and Microanalysis* (2021). DOI: 10.1017/S1431927621010163.

223. Radhakrishnan, M.; Kombaiah, B.; Bachhav, M. N.; Nizolek, T. J.; Wang, Y. Q.; Knezevic, M.; Mara, N.; Anderoglu, O. Layer Dissolution in Accumulative Roll Bonded Bulk Zr/Nb Multilayers Under Heavy-Ion Irradiation. *Journal of Nuclear Materials* (2021). DOI: 10.1016/J.Jnucmat.2021.153315.

224. Rajak, P.; Nakano, A.; Vashishta, P.; Kalia, R. Mechanical Behavior of Ultralight Nickel Metamaterial. *Applied Physics Letters* (2021). DOI: 10.1063/5.0031806.

225. Rana, R.; Long, D.; Kotula, P.; Xu, Y.; Olson, D.; Galipaud, J.; Lemogne, T.; Tysoe, W. T. Insights into the Mechanism of The Mechanochemical Formation of Metastable Phases. *Acs Applied Materials & Interfaces* (2021). DOI: 10.1021/Acsami.0c18980.

226. Reis, M.; Gusev, F.; Taylor, N. G.; Chung, S. H.; Verber, M. D.; Lee, Y. Z.; Isayev, O.; Leibfarth, F. A. Machine-Learning-Guided Discovery of F-19 Mri Agents Enabled by Automated Copolymer Synthesis. *Journal of The American Chemical Society* (2021). DOI: 10.1021/Jacs.1c08181.

227. Liu, R.; Lee, J.; Tchoe, Y.; Pre, D.; Bourhis, A. M.; D'antonio-Chronowska, A.; Robin, G.; Lee, S. H.; Ro, Y. G.; Vatsyayan, R.; Tonsfeldt, K. J.; Hossain, L. A.; Phipps, M. L.; Yoo, J.; Nogan, J.; Martinez, J. S.; Frazer, K. A.; Bang, A. G.; Dayeh, S. A. Ultra-Sharp Nanowire Arrays Natively Permeate, Record, and Stimulate Intracellular Activity in Neuronal and Cardiac Networks. *Advanced Functional Materials* (2021). DOI: 10.1002/Adfm.202108378.

228. Richards, C. G.; Williams, D. J.; Hehlen, M. P.; Hunter, J. F.; Wiggins, B. W. Optically Translucent Bafci:Sm2+ Scintillating Micro-Particle Composites for Radiation Detection. *Optical Materials Express* (2021). DOI: 10.1002/Adfm.202102311.

229. Riley, C.; De La Riva, A.; Park, J. E.; Percival, S. J.; Benavidez, A.; Coker, E. N.; Aidun, R. E.; Paisley, E. A.; Datye, A.; Chou, S. S. A High Entropy Oxide Designed to Catalyze Co Oxidation Without Precious Metals. *Acs Applied Materials & Interfaces* (2021). DOI: 10.1021/Acsami.0c17446.

230. Riley, C. R.; De La Riva, A.; Ibarra, I. L.; Datye, A. K.; Chou, S. S. Achieving High Ethylene Yield in Non-Oxidative Ethane Dehydrogenation. *Applied Catalysis A-General* (2021). DOI: 10.1016/J.Apcata.2021.118309.

231. Robinson, A. J.; House, G. L.; Morales, D. P.; Kelliher, J. M.; Gallegos-Graves, L. V.; Lebrun, E. S.; Davenport, K. W.; Palmieri, F.; Lohberger, A.; Bregnard, D.; Estoppey, A.; Buffi, M.; Paul, C.; Junier, T.; Herve, V.; Cailleau, G.; Lupini, S.; Nguyen, H. N.; Zheng, A. O.; Gimenes, L. J.; Bindschedller, S.; Rodrigues, D. F.; Werner, J. H.; Young, J. D.; Junier, P.; G Chain, P. S. Widespread Bacterial Diversity Within The Bacteriome of Fungi. *Communications Biology* (2021). DOI: 10.1038/S42003-021-02693-Y.

232. Rodriguez-Hernandez, B.; Nelson, T.; Oldani, N.; Martinez-Mesa, A.; Uranga-Pina, L.; Segawa, Y.; Tretiak, S.; Itami, K.; Fernandez-Alberti, S. Exciton Spatial Dynamics and Self-Trapping in Carbon Nanocages. *Journal of Physical Chemistry Letters* (2021). DOI: 10.1021/Acs.Jpclett.0c03364.

233. Rollins, D. S.; Easterling, C. P.; Zeppuhar, A. N.; Krawchuck, J. A.; Dreier, T. A.; Watt, J.; Huber, D. L.; Taylor, M. K. Templated Synthesis Enhances the Cobalt Adsorption Capacity of A Porous Organic Polymer. *Nanoscale* (2022). DOI: 10.1039/D1nr06821k.

234. Rouhi, S.; Ozdemir, M.; Ekmekcioglu, M.; Yigen, S.; Demirhan, Y.; Szerling, A.; Kosiel, K.; Kozubal, M.; Kruszka, R.; Prokaryn, P.; Ertugrul, M.; Reno, J. L.; Aygun, G.; Ozyuzer, L. in-Situ Thin Film Copper-Copper Thermocompression Bonding for Quantum Cascade Lasers. *Journal*

of Materials Science-Materials in Electronics (2021). DOI: 10.1007/S10854-021-06109-9.

235. Saadat, Y.; Kim, K.; Foudazi, R. Initiator-Dependent Kinetics of Lyotropic Liquid Crystal-Templated Thermal Polymerization Dagger. *Polymer Chemistry* (2021). DOI: 10.1039/D1py00127b.

236. Salvador, F. E.; Miller, V.; Shimada, K.; Wang, C.-H.; Wright, J.; Das, M.; Chen, Y.-P.; Chen, Y.-S.; Sheehan, C.; Xu, W.; Rubasinghege, G.; Gao, W.-Y. Mechanochemistry of Group 4 Element-Based Metal-Organic Frameworks. *Inorganic Chemistry* (2021). DOI: 10.1021/Acs.Inorgchem.1c02704.

237. Saper, G.; Tsitkov, S.; Katira, P.; Hess, H. Robotic End-to-End Fusion of Microtubules Powered by Kinesin. *Science Robotics* (2021). DOI: 10.1126/Scirobotics.Abj7200.

238. Sapkota, K. R.; Leonard, F.; Talin, A. A.; Gunning, B. P.; Kazanowska, B. A.; Jones, K. S.; Wang, G. T. Ultralow Voltage Gan Vacuum Nanodiodes in Air. *Nano Letters* (2021). DOI: 10.1021/Acs.Nanolett.0c03959.

239. Schultz, P. A.; Hjalmarson, H. P.; Berg, M.; Bussmann, E.; Scrymgeour, D. A.; Ohta, T.; Moore, C. H. First-Principles Calculations of Metal Surfaces. Ii. Properties of Low-Index Platinum Surfaces Toward Understanding Electron Emission. *Physical Review B* (2021). DOI: 10.1103/Physrevb.103.195427.

240. Schultz, P. A.; Van Ginhoven, R. M.; Edwards, A. H. Theoretical Study of Intrinsic Defects in Cubic Silicon Carbide 3c-Sic. *Physical Review B* (2021). DOI: 10.1103/Physrevb.103.195202.

241. Scott, E. A.; Braun, J. L.; Hattar, K.; Sugar, J. D.; Gaskins, J. T.; Goorsky, M.; King, S. W.; Hopkins, P. E. Probing Thermal Conductivity of Subsurface, Amorphous Layers in Irradiated Diamond. *Journal of Applied Physics* (2021). DOI: 10.1063/5.0038972.

242. Scott, E. A.; Hattar, K.; Lang, E. J.; Aryana, K.; Gaskins, J. T.; Hopkins, P. E. Reductions in The Thermal Conductivity of Irradiated Silicon Governed by Displacement Damage. *Physical Review B* (2021). DOI: 10.1557/S43578-021-00426-9.

243. Senanayake, M.; Aryal, D.; Grest, G. S.; Perahia, D. Interfacial Response and Structural Adaptation of Structured Polyelectrolyte Thin Films. *Macromolecules* (2021). DOI: 10.1021/Acs.Macromol.0c02838.

244. Senanayake, M.; Perahia, D.; Grest, G. S. Effects of Interaction Strength of Associating Groups on Linear and Star Polymer Dynamics. *Journal of Chemical Physics* (2021). DOI: 10.1063/5.0038097.

245. Seo, S.; Hayami, S.; Su, Y.; Thomas, S. M.; Ronning, F.; Bauer, E. D.; Thompson, J. D.; Lin, S.-Z.; Rosa, P. F. S. Spin-Texture-Driven Electrical Transport in Multi-Q Antiferromagnets. *Communications Physics* (2021). DOI: 10.1038/S42005-021-00558-8.

246. Shang, Z.; Fan, C.; Ding, J.; Xue, S.; Gabriel, A.; Shao, L.; Voisin, T.; Wang, Y. M.; Niu, T.; Li, J.; De La Rubia, T. D.; Wang, H.; Zhang, X. Heavy Ion Irradiation Response of An Additively Manufactured 316ln Stainless Steel. *Journal of Nuclear Materials* (2021). DOI: 10.1016/J.Jnucmat.2020.152745.

247. Sharma, S.; Andrade, G. A.; Maurya, S.; Popov, I. A.; Batista, E. R.; Davis, B. L.; Mukundan, R.; Smythe, N. C.; Tondreau, A. M.; Yang, P.; Gordon, J. C. Iron-Iminopyridine Complexes As Charge Carriers for Non-Aqueous Redox Flow Battery Applications. *Energy Storage Materials* (2021). DOI:10.1016/J.ensm.2021.01.035.

248. Sharma, Y.; Mazza, A. R.; Musico, B. L.; Skoropata, E.; Nepal, R.; Jin, R.; Ievlev, A., V; Collins, L.; Gai, Z.; Chen, A.; Brahlek, M.; Keppens, V.; Ward, T. Z. Magnetic Texture in Insulating Single Crystal High Entropy Oxide Spinel Films. *Acs Applied Materials & Interfaces* (2021). DOI: 10.1021/Acsami.1c01344.

249. Sharma, Y.; Paudel, B.; Lee, J.; Choi, W. S.; Yang, Z.; Wang, H.; Du, Y.; Kang, K. T.; Pilania, G.; Chen, A. Tuning Magnetic and Optical Properties Through Strain in Epitaxial $Lacro_3$ Thin Films. *Applied Physics Letters* (2021). DOI: 10.1063/5.0058678.

250. Sheely, A.; Gifford, B.; Tretiak, S.; Bishop, A. Tunable Optical Features of Graphene Quantum Dots from Edge Functionalization. *Journal of Physical Chemistry C* (2021). DOI: 10.1021/Acs.Jpcc.1c00537.

251. Sheil, R.; Butts, D.; Jungjohann, K.; Yoo, J.; Dunn, B.; Chang, J. P. Plasma Enhanced Atomic Layer Deposition of Thin Film $Li_{1+X}mn_{2-X}o_4$ for Realization of All Solid-State 3d Lithium-Ion Microbatteries. *Journal of Vacuum Science & Technology A* (2021). DOI: 10.1116/6.0000644.

252. Sifain, A. E.; Lystrom, L.; Messerly, R. A.; Smith, J. S.; Nebgen, B.; Barros, K.; Tretiak, S.; Lubbers, N.; Gifford, B. J. Predicting Phosphorescence Energies and Inferring Wave Function Localization with Machine Learning. *Chemical Science* (2021). DOI: DOI.Org/10.1039/D1sc02136b.

253. Singh, M. K.; Ghosh, C.; Miller, B.; Carter, C. B. Direct Visualization of The Earliest Stages of Crystallization. *Microscopy and Microanalysis* (2021). DOI: 10.1017/S1431927621000441.

254. Sirica, N.; Orth, P. P.; Scheurer, M. S.; Dai, Y. M.; Lee, M.-C.; Padmanabhan, P.; Mix, L. T.; Teitelbaum, S. W.; Trigo, M.; Zhao, L. X.; Chen, G. F.; Xu, B.; Yang, R.; Shen, B.; Hu, C.; Lee, C.-C.; Lin, H.; Cochran, T. A.; Trugman, S. A.; Zhu, J.-X.; Hasan, M. Z.; Ni, N.; Qiu, X. G.; Taylor, A. J.; Yarotski, D. A.; Prasankumar, R. P. Nature Materials 2021, 21 (1), 62–66. Photocurrent-Driven Transient Symmetry Breaking in The Weyl Semimetal Taas. *Nature Materials* (2021). DOI: 10.1038/S41563-021-01126-9.

255. Sirica, N. S.; Prasankumar, R. P. Shaking Up Topology with Light. *Nature Materials* (2021). DOI: 10.1038/S41563-021-00938-Z.

256. Smallwood, C. L.; Ulbricht, R.; Day, M. W.; Schroeder, T.; Bates, K. M.; Autry, T. M.; Diederich, G.; Bielejec, E.; Siemens, M. E.; Cundiff, S. T. Hidden Silicon-Vacancy Centers in Diamond. *Physical Review Letters* (2021). DOI: 10.1103/Physrevlett.126.213601.

257. Smith, J. S.; Nebgen, B.; Mathew, N.; Chen, J.; Lubbers, N.; Burakovsky, L.; Tretiak, S.; Nam, H. A.; Germann, T.; Fensin, S.; Barros, K. Automated Discovery of a Robust Interatomic Potential for Aluminum. *Nature Communications* (2021). DOI: 10.1038/S41467-021-21376-0.

258. Soh, D.; Chatterjee, E.; Eichenfield, M. High-Fidelity State Transfer Between Leaky Quantum Memories.*Physical Review Research* (2021). DOI: 10.1103/Physrevresearch.3.033027.

259. Song, H.; Freixas, V. M.; Fernandez-Alberti, S.; White, A. J.; Zhang, Y.; Mukamel, S.; Govind, N.; Tretiak, S. An Ab Initio Multiple Cloning Method for Non-Adiabatic Excited-State Molecular Dynamics in Nwchem. *Journal of Chemical Theory and Computation* (2021). DOI: 10.1021/Acs.Jctc.1c00131.

260. Song, H.; Nam, Y.; Keefer, D.; Garavelli, M.; Mukamel, S.; Tretiak, S. Nonadiabatic Molecular Dynamics Study of The Relaxation Pathways of Photoexcited Cyclooctatetraene. *Journal of Physical Chemistry Letters* (2021). DOI: 10.1021/Acs.Jpclett.1c01397.

261. Song, J.; Zhuang, S.; Martin, M.; Ortiz-Flores, L. A.; Paudel, B.; Yarotski, D.; Hu, J.; Chen, A.; Huey, B. D. Interfacial-Strain-Controlled Ferroelectricity in Self-Assembled $Bifeo_3$ Nanostructures. *Advanced Functional Materials* (2021). DOI: 10.1002/Adfm.202102311.

262. Song, Y.; Perez, C.; Esteves, G.; Lundh, J. S.; Saltonstall, C. B.; Beechem, T. E.; Yang, J. I.; Ferri, K.; Brown, J. E.; Tang, Z.; Maria, J.-P.; Snyder, D. W.; Olsson, R. H., Iii; Griffin, B. A.; Trolier-Mckinstry, S. E.; Foley, B. M.; Choi, S. Thermal Conductivity of Aluminum Scandium Nitride for 5g Mobile Applications and Beyond. *Acs Applied Materials & Interfaces* (2021). DOI: 10.1021/Acsami.1c02912.

263. Srivastava, I.; Roberts, S. A.; Clemmer, J. T.; Silbert, L. E.; Lechman, J. B.; Grest, G. S. Jamming of Bidisperse Frictional Spheres. *Physical Review Research* (2021). DOI: 10.1103/Physrevresearch.3.L032042.

264. Srivastava, I.; Silbert, L. E.; Grest, G. S.; Lechman, J. B. Viscometric Flow of Dense Granular Materials Under Controlled Pressure and Shear Stress. *Journal of Fluid Mechanics* (2021). DOI: 10.1017/Jfm.2020.811.

265. Srivastava, I.; Silbert, L. E.; Lechman, J. B.; Grest, G. S. Flow and Arrest in Stressed Granular Materials. *Soft Matter* (2021). DOI: 10.1039/D1sm01344k.

266. Stangebye, S.; Zhang, Y.; Gupta, S.; Hosseinian, E.; Yu, F.; Barr, C.; Hattar, K.; Pierron, O.; Zhu, T.; Kacher, J. Grain Growth of Nanocrystalline Aluminum Under Tensile Deformation: A Combined in-Situ Tem and Atomistic Study. *Materialia* (2021). DOI: 10.1016/J.Mtla.2021.101068.

267. Startt, J.; Deo, C.; Dingreville, R. Vacancy Surface Migration Mechanisms in Dilute Nickel-Chromium Alloys. *Scripta Materialia* (2021). DOI: 10.1016/J.Scriptamat.2021.113998.

268. Startt, J.; Dingreville, R.; Raiman, S.; Deo, C. An Electronic Origin to The Oscillatory Segregation Behavior in Ni-Cr and Other Bcc Defects in Fcc Metals. *Acta Materialia* (2021). DOI: 10.1038/S41467-021-21332-Y.

269. Startt, J.; Dingreville, R.; Raiman, S. S.; Deo, C. Ab-Initio Investigation of The Effect of Adsorbed Salts on Segregation of Cr at The Ni (100) Surface. *Applied Surface Science* (2021). DOI: 10.1016/J.Apsusc.2021.149836.

270. Stevens, M. J. Simulation of Polymerization Induced Phase Separation in Model Thermosets. *Journal of Chemical Physics* (2021). DOI: 10.1063/5.0061654.

271. Stevenson, S. R.; Delker, C. J.; Nordquist, C. D.; Solomon, O. M.; Johnson-Wilke, R. L.; Ballance, M. H.; Sandoval, R. L.; Harris, C. T. Characterization and Modeling of Two-Port Wideband

Resistance Calibration Standards. *Ieee Microwave and Wireless Components Letters* (2021). DOI: 10.1109/Lmwc.2021.3054577.

272. Stromberg, Z. R.; Phipps, M. L.; Magurudeniya, H. D.; Pedersen, C. A.; Rajale, T.; Sheehan, C. J.; Courtney, S. J.; Bradfute, S. B.; Hraber, P.; Rush, M. N.; Kubicek-Sutherland, J. Z.; Martinez, J. S. Formulation of Stabilizer-Free, Nontoxic Plga and Elastin-Plga Nanoparticle Delivery Systems. *International Journal of Pharmaceutics* (2021). DOI: 10.1016/J.Ijpharm.2021.120340.

273. Studenikin, S.; Korkusinski, M.; Bogan, A.; Gaudreau, L.; Austing, D. G.; Sachrajda, A. S.; Tracy, L.; Reno, J.; Hargett, T. Single-Hole Physics in Gaas/Algaas Double Quantum Dot System with Strong Spin-Orbit Interaction. *Semiconductor Science and Technology* (2021). DOI: 10.1088/1361-6641/Abe42d.

274. Su, R.; Neffati, D.; Cho, J.; Shang, Z.; Zhang, Y.; Ding, J.; Li, Q.; Xue, S.; Wang, H.; Kulkarni, Y.; Zhang, X. High-Strength Nanocrystalline Intermetallics with Room Temperature Deformability Enabled by Nanometer Thick Grain Boundaries. *Science Advances* (2021). DOI: 10.1126/Sciadv.Abc8288.

275. Su, R.; Neffati, D.; Li, Q.; Xue, S.; Fan, C.; Cho, J.; Zhang, Y.; Li, J.; Wang, H.; Kulkarni, Y.; Zhang, X. Ultra-High Strength and Plasticity Mediated by Partial Dislocations and Defect Networks: Part Ii: Layer Thickness Effect. *Acta Materialia* (2021). DOI: 10.1016/J.Actamat.2020.116494.

276. Su, R.; Neffati, D.; Zhang, Y.; Cho, J.; Li, J.; Wang, H.; Kulkarni, Y.; Zhang, X. The Influence of Stacking Faults on Mechanical Behavior of Advanced Materials. *Materials Science and Engineering A-Structural Materials Properties Microstructure and Processing* (2021). DOI: 10.1016/J.Msea.2020.140696.

277. Sukharev, M.; Roslyak, O.; Piryatinski, A. Second-Harmonic Generation in Nonlinear Plasmonic Lattices Enhanced by Quantum Emitter Gain Medium. *Journal of Chemical Physics* (2021). DOI: 10.1063/5.0037453.

278. Mohottalalage, S. S.; Aryal, D.; Thurston, B. A.; Grest, G. S.; Perahia, D. Effects of Ionic Group Distribution on the Structure and Dynamics of Amorphous Polymer Melts. *Macromolecules* (2021). DOI: 10.1021/Acs.Macromol.1c02141.

279. Surendran, M.; Chen, H.; Zhao, B.; Thind, A. S.; Singh, S.; Orvis, T.; Zhao, H.; Han, J.-K.; Htoon, H.; Kawasaki, M.; Mishra, R.; Ravichandran, J. Epitaxial Thin Films of a Chalcogenide Perovskite. *Chemistry of Materials* (2021). DOI: 10.1021/Acs.Chemmater.1c02202.

280. Ahmed, S. Z.; Ahmed, I.; Mia, M. B.; Jaidye, N.; Kim, S. Ultra-High Extinction Ratio Polarization Beam Splitter with Extreme Skin-Depth Waveguide. *Optics Letters* (2021). DOI: 10.1364/Ol.420824.

281. Tai, C.-T.; Chiu, P.-Y.; Liu, C.-Y.; Kao, H.-S.; Harris, C. T.; Lu, T.-M.; Hsieh, C.-T.; Chang, S.-W.; Li, J.-Y. Strain Effects on Rashba Spin-Orbit Coupling of 2d Hole Gases in Gesn/Ge Heterostructures.*Advanced Materials* (2021). DOI: 10.1002/Adma.202007862.

282. Tang, J.; Cheng, T.; Wang, Y.; Hu, L.; Hong, M.; Qin, W.; Cai, G.; Jiang, C.; Ren, F. Constructing High-Performance Radiation-Resistant Ternary Ysz-Mgo-Cnt Nanocomposites Via Tailored Nanostructures. *Journal of The European Ceramic Society* (2021). DOI:

10.1016/J.Jeurceramsoc.2021.04.029.

283. Tang, Z.; Watkins, E. B.; Clayton, S. M.; Currie, S. A.; Fellers, D. E.; Hassan, M. T.; Hooks, D. E.; Ito, T. M.; Lawrence, S. K.; Macdonald, S. W. T.; Makela, M.; Morris, C. L.; Neukirch, L. P.; Saunders, A.; O'shaughnessy, C. M.; Cude-Woods, C.; Choi, J. H.; Young, A. R.; Zeck, B. A.; Gonzalez, F.; Liu, C. Y.; Floyd, N. C.; Hickerson, K. P.; Holley, A. T.; Johnson, B. A.; Lambert, J. C.; Pattie, R. W. Ultracold Neutron Properties of The Eljen-299-02d Deuterated Scintillator. *Review of Scientific Instruments* (2021). DOI:10.1063/5.0030972.

284. Tappan, B. C.; Steiner, S. A., Iii; Dervishi, E.; Mueller, A. H.; Scott, B. L.; Sheehan, C.; Luther, E. P.; Lichthardt, J. P.; Dirmyer, M. R. Monolithic Nanoporous Gold Foams with Catalytic Activity for Chemical Vapor Deposition Growth of Carbon Nanostructures. *Acs Applied Materials & Interfaces* (2021). DOI: 10.1021/Acsami.0c17624.

285. Taylor, C. A.; Lang, E.; Kotula, P. G.; Goeke, R.; Snow, C. S.; Wang, Y.; Hattar, K. Helium Bubbles and Blistering in A Nanolayered Metal/Hydride Composite. *Materials* (2021). DOI: 10.3390/Ma14185393.

286. Teplukhin, A.; Kendrick, B. K.; Mniszewski, S. M.; Zhang, Y.; Kumar, A.; Negre, C. F. A.; Anisimov, P. M.; Tretiak, S.; Dub, P. A. Computing Molecular Excited States on a D-Wave Quantum Annealer. *Scientific Reports* (2021). DOI: 10.1038/S41598-021-98331-Y.

287. Thakral, S.; Kim, K. Small-Angle Scattering for Characterization of Pharmaceutical Materials. *Trac-Trends in Analytical Chemistry* (2021). DOI: 10.1016/J.Trac.2020.116144.

288. Thapa, A.; Poudel, Y. R.; Guo, R.; Jungjohann, K. L.; Wang, X.; Li, W. Direct Synthesis of Micropillars of Vertically Aligned Carbon Nanotubes on Stainless-Steel and Their Excellent Field Emission Properties. *Carbon* (2021). DOI: 10.1016/J.Carbon.2020.08.081.

289. Thomas, C. J.; Fonseca, J. J.; Spataru, C. D.; Robinson, J. T.; Ohta, T. Electronic Structure and Stacking Arrangement of Tungsten Disulfide at The Gold Contact. *Acs Nano* (2021). DOI: 10.1021/Acsnano.1c06676.

290. Titze, M.; Pacheco, J. L.; Byers, T.; Van Deusen, S. B.; Perry, D. L.; Weathers, D.; Bielejec, E. S. Evaluation of The Accuracy of Stopping and Range of Ions in Matter Simulations Through Secondary Ion Mass Spectrometry and Rutherford Backscattering Spectrometry for Low Energy Heavy Ion Implantation. *Journal of Vacuum Science & Technology A* (2021). DOI: 10.1016/J.Actamat.2021.117302.

291. Titze, M.; Perry, D. L.; Auden, E. A.; Pacheco, J. L.; Abraham, J. B. S.; Bielejec, E. S. Lithium Source for Focused Ion Beam Implantation and Analysis. *Journal of Vacuum Science & Technology B* (2021). DOI: 10.1116/6.0000645.

292. Tkachenko, N. V; Sud, J.; Zhang, Y.; Tretiak, S.; Anisimov, P. M.; Arrasmith, A. T.; Coles, P. J.; Cincio, L.; Dub, P. A. Correlation-Informed Permutation of Qubits for Reducing Ansatz Depth in The Variational Quantum Eigensolver. *Prx Quantum* (2021). DOI: 10.1103/Prxquantum2.020337.

293. Rajale, T.; Miner, J. C.; Michalczyk, R.; Phipps, M. L.; Schmidt, J. G.; Gilbertson, R. D.; Williams, R. F.; Strauss, C. E.; Martinez, J. S. Conformational Control Via Sequence for A Heteropeptoid

in Water: Coupled Nmr and Rosetta Modelling. *Royal Society of Chemistry Chemical Communications* (2021). DOI: 10.1039/D1cc01992a.

294. Tsai, H.; Shrestha, S.; Vila, R. A.; Huang, W.; Liu, C.; Hou, C.-H.; Huang, H.-H.; Wen, X.; Li, M.; Wiederrecht, G.; Cui, Y.; Cotlet, M.; Zhang, X.; Ma, X.; Nie, W. Bright and Stable Light-Emitting Diodes Made with Perovskite Nanocrystals Stabilized in Metal-Organic Frameworks. *Nature Photonics* (2021). DOI: 10.1038/S41566-021-00857-0.

295. Tsymbalov, E.; Shi, Z.; Dao, M.; Suresh, S.; Li, J.; Shapeev, A. Machine Learning for Deep Elastic Strain Engineering of Semiconductor Electronic Band Structure and Effective Mass. *Npj Computational Materials* (2021). DOI: 10.1038/S41524-021-00538-0.

296. Turner, E. M.; Campbell, Q.; Pizarro, J.; Yang, H.; Sapkota, K. R.; Lu, P.; Baczewski, A. D.; Wang, G. T.; Jones, K. S. Controlled Formation of Stacked Si Quantum Dots in Vertical Sige Nanowires. *Nano Letters* (2021). DOI: 10.1021/Acs.Nanolett.1c01670.

297. Uliana, A. A.; Bui, N. T.; Kamcev, J.; Taylor, M. K.; Urban, J. J.; Long, J. R. Ion-Capture Electrodialysis Using Multifunctional Adsorptive Membranes. *Science* (2021). DOI: 10.1126/Science.Abf5991.

298. Mapara, V.; Stevens, C. E.; Paul, J.; Barua, A.; Reno, J. L.; Mcgill, S. A.; Hilton, D. J.; Karaiskaj, D. Multidimensional Spectroscopy of Magneto-Excitons at High Magnetic Fields. *Journal of Chemical Physics* (2021). DOI: 10.1063/5.0070113.

299. Vabishchevich, P. P.; Vaskin, A.; Karl, N.; Reno, J. L.; Sinclair, M. B.; Staude, I.; Brener, I. Ultrafast All-Optical Diffraction Switching Using Semiconductor Metasurfaces. *Applied Physics Letters* (2021). DOI: 10.1063/5.0049585.

300. Vaidya, S.; Benalcazar, W. A.; Cerjan, A.; Rechtsman, M. C. Point Defect Localized Bound States in The Continuum in Photonic Crystals and Structured Fibers. *Physical Review Letters* (2021). DOI: 10.1103/Physrevlett.127.023605.

301. Valente, D. C. A.; Do Casal, M. T.; Barbatti, M.; Niehaus, T. A.; Aquino, A. J. A.; Lischka, H.; Cardozo, T. M. Excitonic and Charge Transfer Interactions in Tetracene Stacked and T-Shaped Dimers. *Journal of Chemical Physics* (2021). DOI: 10.1063/5.0033272.

302. Vangordon, M. R.; Prignano, L. A.; Dempski, R. E.; Rick, S. W.; Rempe, S. B. Channelrhodopsin C1c2: Photocycle Kinetics and Interactions Near the Central Gate. *Biophysical Journal* (2021). DOI: 10.1016/J.Bpj.2021.03.002.

303. Vaskin, A.; Liu, S.; Addamane, S.; Vabishchevich, P. P.; Yang, Y.; Balarishnan, G.; Sinclair, M. B.; Pertsch, T.; Brener, I.; Staude, I. Manipulation of Quantum Dot Emission with Semiconductor Metasurfaces Exhibiting Magnetic Quadrupole Resonances. *Optics Express* (2021). DOI: 10.1364/Oe.414011.

304. Vizoso, D.; Kosmidou, M.; Balk, T. J.; Hattar, K.; Deo, C.; Dingreville, R. Size-Dependent Radiation Damage Mechanisms in Nanowires and Nanoporous Structures. *Acta Materialia* (2021). DOI:10.1016/J.Actamat.2021.117018.

305. Kazanowska, B. A.; Sapkota, K. R.; Lu, P.; Talin, A. A.; Bussmann, E.; Ohta, T.; Gunning, B. P.; Jones, K. S.; Wang, G. T. Fabrication and Field Emission Properties of Vertical, Tapered Gan

Nanowires Etched Via Phosphoric Acid. *Nanotechnology* (2021). DOI: 10.1088/1361-6528/Ac2981.

306. Wang, F.; Yan, X.; Chen, X.; Snyder, N.; Nastasi, M.; Hattar, K.; Cui, B. Pulsed Electric Current Joining of Oxide-Dispersion-Strengthened Austenitic Steels. *Journal of Materials Science* (2021). DOI: 10.1007/S10853-021-06495-9.

307. Wang, J.; Jiang, Y.; Zhao, T.; Dun, Z.; Miettinen, A. L.; Wu, X.; Mourigal, M.; Zhou, H.; Pan, W.; Smirnov, D.; Jiang, Z. Magneto-Transport Evidence for Strong Topological Insulator Phase in $Zrte_5$. *Nature Communications* (2021). DOI: 10.1038/S41467-021-27119-5.

308. Wang, J.; Knezevic, M.; Jain, M.; Pathak, S.; Beyerlein, I. J. Role of Interface-Affected Dislocation Motion on the Strength of Mg/Nb Nanolayered Composites Inferred by Dual-Mode Confined Layer Slip Crystal Plasticity. *Journal of The Mechanics and Physics of Solids* (2021). DOI: 10.1016/J.Jmps.2021.104421.

309. Wang, J.; O'connor, T. C.; Grest, G. S.; Zheng, Y.; Rubinstein, M.; Ge, T. Diffusion of Thin Nanorods in Polymer Melts. *Macromolecules* (2021). DOI: 10.1021/Acs.Macromol.1c00989.

310. Weight, B. M.; Gifford, B. J.; Tretiak, S.; Kilina, S. Interplay Between Electrostatic Properties of Molecular Adducts and Their Positions at Carbon Nanotubes. *Journal of Physical Chemistry C* (2021). DOI: 10.1021/Acs.Jpcc.0c10157.

311. Weight, B. M.; Sifain, A. E.; Gifford, B. J.; Kilin, D.; Kilina, S.; Tretiak, S. Coupling Between Emissive Defects on Carbon Nanotubes: Modeling Insights. *Journal of Physical Chemistry Letters* (2021). DOI: 10.1021/Acs.Jpclett.1c01631.

312. Wheeler, J. M.; Harvey, C.; Li, N.; Misra, A.; Mara, N. A.; Maeder, X.; Michler, J.; Pathak, S. High Temperature Nanoindentation of Cu-Tin Nanolaminates. *Materials Science and Engineering A-Structural Materials Properties Microstructure and Processing* (2021). DOI: 10.1016/J.Msea.2020.140522.

313. White, B. C.; Garland, A.; Alberdi, R.; Boyce, B. L. Interpenetrating Lattices with Enhanced Mechanical Functionality. *Additive Manufacturing* (2021). DOI: 10.1016/J.Addma.2020.101741.

314. Wijesinghe, S.; Perahia, D.; Ge, T.; Salerno, K. M.; Grest, G. S. Stress Relaxation of Comb Polymer Melts. *Tribology Letters* (2021). DOI: 10.1007/S11249-021-01432-Y.

315. Woo, S.; Yoo, J.; Magginetti, D. J.; Bilgin, I.; Kar, S.; Yoon, H. P.; Yoon, Y. Resolving Surface Potential Variation in Ge/Mos_2 Heterostructures with Kelvin Probe Force Microscopy. *Aip Advances* (2021). DOI: 10.1063/5.0075599.

316. Wu, Y.; Shen, Y.; Addamane, S.; Reno, J. L.; Williams, B. S. Tunable Quantum-Cascade Vecsel Operating at 1.9 Thz. *Optics Express* (2021). DOI: 10.1364/Oe.438636.

317. Wu, Y.; Iwase, K.; Harada, T.; Nakanishi, S.; Kamiya, K. Sn Atoms on Cu Nanoparticles for Suppressing Competitive H-2 Evolution in Co_2 Electrolysis. *Acs Applied Nano Materials* (2021). DOI: 10.1021/Acsanm.1c00514.

318. Wang, X.; Kim, Y.; Baldwin, J. K.; Jones, A. C.; Jeong, J.; Kang, K. T.; Chen, A.; Yoo, J. Enhanced

Van Der Waals Epitaxy of Germanium by Out-of-Plane Dipole Moment Induced From Transferred Graphene on Tin/Aln Multilayers. *Journal of Applied Physics* (2021). DOI: 10.1063/5.0065306.

319. Wu, Y.; Addamane, S.; Reno, J. L.; Williams, B. S. Multi-Mode Lasing in Terahertz Metasurface Quantum-Cascade Vecsels. *Applied Physics Letters* (2021). DOI: 10.1063/5.0061391.

320. Yadav, D.; Zhao, D.; Baldwin, J. K.; Devaraj, A.; Demkowicz, M. J.; Xie, K. Y. Persistence of Crystal Orientations Across Sub-Micron-Scale Super-Grains in Self-Organized Cu-W Nanocomposites. *Scripta Materialia* (2021). DOI: 10.1016/J.Scriptamat.2020.113677.

321. Kim, Y.; Tutchton, R.; Liu, R.; Krylyuk, S.; Zhu, J.-X.; Davydov, A. V.; Hong, Y. J.; Yoo, J. Single-Layer Dititanium Oxide Ti_2o Moene: Multifunctional Promises for Electride, Anode Materials, and Superconductor. *Journal of Physical Chemistry Letters* (2021). DOI: 10.1021/Acs.Jpclett.0c03397.

322. Kim, Y.; Tutchton, R.; Liu, R.; Krylyuk, S.; Zhu, J.-X.; Davydov, A. V.; Hong, Y. J.; Yoo, J. Low Barrier Height in A Zno Nanorods $Nbse_2$ Heterostructure Prepared by Van Der Waals Epitaxy. *Apl Materials* (2021). DOI: 10.1063/5.0052596.

323. Wang, Y.; Dong, H.; Katyal, N.; Hao, H.; Liu, P.; Celio, H.; Henkelman, G.; Watt, J.; Mitlin, D. Sodium-Antimony-Telluride Intermetallic Allows Sodium Metal Cycling at 100% Depth of Discharge and As Anode-Free Metal Battery. *Advanced Materials* (2021). DOI: 10.1002/Adma.202106005.

324. Young, J. M.; Byers, T. A.; Lang, E. J.; Singh, S.; Glass, G. A.; Hattar, K.; Rout, B. Synthesis of Magnesiowustite Nanocrystallites Embedded in An Amorphous Silicate Matrix Via Low Energy Multiple Ion Implantations. *Planetary and Space Science* (2021). DOI: 10.1016/J.Pss.2021.105319.

325. Yu, R.; Hu, H.; Nica, E. M.; Zhu, J.-X.; Si, Q. Orbital Selectivity in Electron Correlations and Superconducting Pairing of Iron-Based Superconductors. *Frontiers in Physics* (2021). DOI: 10.3389/Fphy.2021.578347.

326. Yuan, L.; Jeong, J.; Kwock, K. W. C.; Yanev, E. S.; Grandel, M.; Rhodes, D. A.; Luk, T. S.; Schuck, P. J.; Yarotski, D.; Hone, J. C.; Brener, I.; Prasankumar, R. P. Manipulation of Exciton Dynamics in Single-Layer Wse_2 Using a Toroidal Dielectric Metasurface. *Nano Letters* (2021). DOI: 10.1021/Acs.Nanolett.1c03189.

327. Yue Shen, A. D. K., Mohammad Shahili, Christopher A. Curwen, Sadhvikas Addamane, John L. Reno, and Benjamin S. Williams. Thz Time-Domain Characterization of Amplifying Quantum-Cascade Metasurface. *Applied Physics Letters* (2022). DOI: 10.1063/5.0067690.

328. Yun, C.; Webb, M.; Li, W.; Wu, R.; Xiao, M.; Hellenbrand, M.; Kursumovic, A.; Dou, H.; Gao, X.; Dhole, S.; Zhang, D.; Chen, A.; Shi, J.; Zhang, K. H. L.; Wang, H.; Jia, Q.; Macmanus-Driscoll, J. L. High Performance, Electroforming-Free, Thin Film Memristors Using Ionic $Na_{0.5}bi_{0.5}tio_3$. *Journal of Materials Chemistry C* (2021). DOI: 10.1039/D1tc00202c.

329. Zade, V.; Makeswaran, N.; Boyce, B. L.; Paraguay-Delgado, F.; Ramana, C., V. Structural and

Mechanical Properties of Nanocrystalline Ga_2o_3 Films Made by Pulsed Laser Deposition onto Transparent Quartz Substrates. *Nano Express* (2021). DOI: 10.1088/2632-959x/Abf3d3.

330. Zapiain, D. M. D. O.; Stewart, J. A.; Dingreville, R. Accelerating Phase-Field-Based Microstructure Evolution Predictions Via Surrogate Models Trained by Machine Learning Methods. *Npj Computational Materials* (2021). DOI: 10.1038/S41524-020-00471-8.

331. Zarnas, P. D.; Boyce, B. L.; Qu, J.; Dingreville, R. Stress-Induced Transition from Vacancy Annihilation to Void Nucleation Near Microcracks. *International Journal of Solids and Structures* (2021). DOI: 10.1016/J.Ijsolstr.2020.12.014.

332. Zhang, J.; Tsai, H.; Nie, W.; Hu, B. Enabling Ac Electroluminescence in Quasi-2d Perovskites by Uniformly Arranging Different-N-Value Nanoplates to Allow Bidirectional Charge Transport. *Nano Energy* (2021). DOI: 10.1016/J.Nanoen.2020.105413.

333. Zhang, R.; Lane, C.; Singh, B.; Nokelainen, J.; Barbiellini, B.; Markiewicz, R. S.; Bansil, A.; Sun, J. Magnetic and F-Electron Effects in $Lanio_2$ and $Ndnio_2$ Nickelates with Cuprate-Like $3d_{x2-Y2}$ Band. *Communications Physics* (2021). DOI: 10.1038/S42005-021-00621-4.

334. Zhang, X.; Wang, F.; Yan, X.; Li, X.-Z.; Hattar, K.; Cui, B. Nanostructured Oxide-Dispersion-Strengthened Cocrfemnni High-Entropy Alloys with High Thermal Stability. *Advanced Engineering Materials* (2021). DOI: 10.1002/Adem.202100291.

335. Zhang, Y.; He, C.; De La Harpe, K.; Goodwin, P. M.; Petty, J. T.; Kohler, B. A Single Nucleobase Tunes Nonradiative Decay in a Dna-Bound Silver Cluster. *Journal of Chemical Physics* (2021). DOI: 10.1063/5.0056836.

336. Zhao, Q. Q.; Boyce, B. L.; Sills, R. B. Micromechanics of Void Nucleation and Early Growth at Incoherent Precipitates: Lattice-Trapped and Dislocation-Mediated Delamination Modes. *Crystals* (2021). DOI: 10.3390/Cryst11010045.

337. Zheng, Y.; Kim, Y.; Jones, A. C.; Olinger, G.; Bittner, E. R.; Bachilo, S. M.; Doorn, S. K.; Weisman, R. B.; Piryatinski, A.; Htoon, H. Quantum Light Emission from Coupled Defect States in Dna-Functionalized Carbon Nanotubes. *Acs Nano* (2021). DOI: 10.1021/Acsnano.1c02709.

338. Zheng, Y.; Weight, B. M.; Jones, A. C.; Chandrasekaran, V.; Gifford, B. J.; Tretiak, S.; Doom, S. K.; Htoon, H. Photoluminescence Dynamics Defined by Exciton Trapping Potential of Coupled Defect States in Dna-Functionalized Carbon Nanotubes. *Acs Nano* (2021). DOI: 10.1021/Acsnano.0c07544.

339. Zhou, Y.; Fernando, K.; Wan, J.; Liu, F.; Shrestha, S.; Tisdale, J.; Sheehan, C. J.; Jones, A. C.; Tretiak, S.; Tsai, H.; Huang, H.; Nie, W. Millimeter-Size All-Inorganic Perovskite Crystalline Thin Film Grown by Chemical Vapor Deposition. *Advanced Functional Materials* (2021). DOI: 10.1002/Adfm.202101058.

340. Zubatiuk, T.; Isayev, O. Development of Multimodal Machine Learning Potentials: Toward a Physics-Aware Artificial Intelligence. *Accounts of Chemical Research* (2021). DOI: 10.1021/Acs.Accounts.0c00868.

341. Zubatiuk, T.; Nebgen, B.; Lubbers, N.; Smith, J. S.; Zubatyuk, R.; Zhou, G.; Koh, C.; Barros, K.;

Isayev, O.; Tretiak, S. Machine-Learned Huckel Theory: Interfacing Physics and Deep Neural Networks. *Journal of Chemical Physics* (2021). DOI: 10.1063/5.0052857.

342. Zubatyuk, R.; Smith, J. S.; Nebgen, B. T.; Tretiak, S.; Isayev, O. Teaching A Neural Network to Attach and Detach Electrons from Molecules. *Nature Communications* (2021). DOI: 10.1038/S41467-021-24904-0.