

## LIST OF MRSEC-SUPPORTED PUBLICATIONS

2021-2022 [241]

March 1, 2021 – February 28, 2022

### IRG-1 [5]

#### a. Primary MRSEC Support that Acknowledge the MRSEC Award DMR-1720256 [2]

1. A.L. Beyerlein, I.J. Beyerlein, Bessel function descriptions of magneto-chiral interactions (DMI)-magnetic and spin flexoelectric skyrmions, *Physica B: Condensed Matter* **613** (2021) 412980. DOI: 10.1016/j.physb.2021.412980
2. D.A. Kitchaev, A. **Van der Ven**, Tuning magnetic antiskyrmion stability in tetragonal inverse Heusler alloys, *Phys. Rev. Mater.* **5** (2021) 124408. DOI: 10.1103/PhysRevMaterials.5.124408

#### b. Partial MRSEC Support that Acknowledge the MRSEC Award DMR-1720256 [3]

3. E. McCalla, E.E. Levin, J.E. Douglas, J.G. Barker, M. Frontzek, W. Tian, R.M. Fernandes, R. **Seshadri**, C. Leighton, Understanding magnetic phase coexistence in Ru<sub>2</sub>Mn<sub>1-x</sub>Fe<sub>x</sub>Sn Heusler alloys: A neutron scattering, thermodynamic, and phenomenological analysis, *Phys. Rev. Mater.* **5** (2021) 064417. DOI: 10.1103/PhysRevMaterials.5.064417
4. P.F. Rottmann, A.T. Polonsky, T. Francis, M.G. Emigh, M. Krispin, G. Rieger, M.P. Echlin, C.G. Levi, T.M. **Pollock**, TriBeam tomography and microstructure evolution in additively manufactured Alnico magnets, *Mater. Today* **49** (2021) 23–34. DOI: 10.1016/j.mattod.2021.05.00323
5. J.L. Zuo, D. Kitchaev, E.C. Schueller, J.D. Bocarsly, R. **Seshadri**, A. **Van der Ven**, S.D. **Wilson**, Magnetoentropic mapping and computational modeling of cycloids and skyrmions in the lacunar spinels GaV<sub>4</sub>S<sub>8</sub> and GaV<sub>4</sub>Se<sub>8</sub>, *Phys. Rev. Mater.* **5** (2021) 54410. DOI: 10.1103/PhysRevMaterials.5.054410

### IRG-2 [10]

#### a. Primary MRSEC Support that Acknowledge the MRSEC Award DMR-1720256 [7]

6. D.J. Grzetic, K.T. Delaney, G.H. **Fredrickson**, Electrostatic manipulation of phase behavior in immiscible charged polymer blends, *Macromolecules* **54** (2021) 2604–2616. DOI: 10.1021/acs.macromol.1c00095
7. S.K. Jain, D. Rawlings, S. Antoine, R.A. **Segalman**, S. Han, Confinement promotes hydrogen bond network formation and Grotthuss proton hopping in ion-conducting block copolymers, *Macromolecules* **55** (2022) 615–622. DOI: 10.1021/acs.macromol.1c01808

8. S.D. Jones, H. Nguyen, P.M. Richardson, Y.-Q. Chen, K.E. Wyckoff, C.J. **Hawker**, R.J. **Clément**, G.H. **Fredrickson**, R.A. **Segalman**, Design of polymeric zwitterionic solid electrolytes with superionic lithium transport, *ACS Cent. Sci.* **8** (2022) 169–175. DOI: 10.1021/acscentsci.1c01260
9. A. Nikolaev, P.M. Richardson, S. Xie, L.C. Llanes, S.D. Jones, O. Nordness, H. Wang, G.C. Bazan, R.A. **Segalman**, R.J. **Clément**, J. **Read de Alaniz**, Role of electron-deficient imidazoles in ion transport and conductivity in solid-state polymer electrolytes, *Macromolecules* **55** (2022) 971–977. DOI: 10.1021/acs.macromol.1c01979
10. N.S. Schauser, G.A. Kliegle, P. Cooke, R.A. **Segalman**, R. **Seshadri**, Database creation, visualization, and statistical learning for polymer Li<sup>+</sup>-electrolyte design, *Chem. Mater.* **33** (2021) 4863–4876. DOI: 10.1021/acs.chemmater.0c04767
11. N.S. Schauser, P.M. Richardson, A. Nikolaev, P. Cooke, G.A. Kliegle, E.M. Susca, K. Johnson, H. Wang, J. **Read de Alaniz**, R. **Clément**, R.A. **Segalman**, Optimum in ligand density for conductivity in polymer electrolytes, *Mol. Syst. Des. Eng.* **6** (2021) 1025–1038. DOI: 10.1039/D1ME00089F
12. A.M. Scheuermann, H. Wakidi, A.T. Lill, S. Oh, L.C. Llanes, C.A. D'Ambra, S. Antoine, M. Wang, M.L. **Chabiny**, T.-Q. **Nguyen**, J. **Read de Alaniz**, C.M. **Bates**, Multiwavelength photodetectors based on an azobenzene polymeric ionic liquid, *ACS Appl. Polym. Mater.* **3** (2021) 5125–5133. DOI: 10.1021/acsapm.1c00884

**b. Partial MRSEC Support that Acknowledge the MRSEC Award DMR-1720256 [3]**

13. A. Abdilla, C.A. D'Ambra, Z. Geng, J.J. Shin, M. Czuczola, D.J. Goldfeld, S. Biswas, J.M. Mecca, S. Swier, T.D. Bekemeier, D.S. Laitar, M.W. Bates, C.M. **Bates**, C.J. **Hawker**, Silicone-based polymer blends: Enhancing properties through compatibilization, *J. Polym. Sci.* **59** (2021) 2114–2128. DOI: 10.1002/pol.20210453
14. H. Li, Y. Zhang, S. Jones, R. **Segalman**, G.G. Warr, R. Atkin, Interfacial nanostructure and friction of a polymeric ionic liquid-ionic liquid mixture as a function of potential at Au(1 1 1) electrode interface, *J. Colloid Interface Sci.* **606**, Part 2 (2022) 1170–1178. DOI: 10.1016/j.jcis.2021.08.067
15. E.M. Thomas, P.H. Nguyen, S.D. Jones, M.L. **Chabiny**, R.A. **Segalman**, Electronic, ionic, and mixed conduction in polymeric systems, *Annu. Rev. Mater. Res.* **51** (2021) 1–20. DOI: 10.1146/annurev-matsci-080619-110405

**IRG-3 [23]**

**a. Primary MRSEC Support that Acknowledge the MRSEC Award DMR-1720256 [8]**

16. M. Areyano, J.A. Booth, D. Brouwer, L.F. Gockowski, M.T. **Valentine**, R.M. **McMeeking**, Suction-controlled detachment of mushroom-shaped adhesive structures, *J. Appl. Mech.* **88** (2021) 031017. DOI: 10.1115/1.4049392

17. A.L. Chau, M.K. Cavanaugh, Y.-T. Chen, A.A. **Pitenis**, A simple contact mechanics model for highly strained aqueous surface gels, *Exp. Mech.* **61** (2021) 699–703.  
DOI: 10.1007/s11340-021-00699-5
18. A.L. Chau, J.M. Urueña, A.A. **Pitenis**, Load-independent hydrogel friction, *Biotribology* **26** (2021) 100183. DOI: 10.1016/j.biortri.2021.100183
19. G.D. Degen, K.C. Cunha, Z.A. Levine, J.H. **Waite**, J-E. **Shea**, Molecular context of dopa influences adhesion of mussel-inspired peptides, *J. Phys. Chem. B* **125** (2021) 9999–10008.  
DOI: 10.1021/acs.jpcb.1c05218
20. Z. Geng, J.J. Shin, Y. Xi, C.J. **Hawker**, Click chemistry strategies for the accelerated synthesis of functional macromolecules, *J. Polym Sci.* **59** (2021) 963–1042.  
DOI: 10.1002/pol.20210126
21. Y. Kwon, J.H. Bernstein, N. Cohen, M.T. **Valentine**, On-demand manufacturing capabilities of mussels enable robust adhesion to geometrically complex surfaces, *ACS Biomater. Sci. & Eng.* **7** (2021) 5099–5106. DOI: 10.1021/acsbiomaterials.1c00845
22. V.J. Shenoy, C.E.R Edwards, M.E. **Helgeson**, M.T. **Valentine**, Design and characterization of a 3D-printed staggered herringbone mixer, *BioTechniques* **70** (2021) 285–289.  
DOI: 10.2144/btn-2021-0009
23. C. Zhang, D.L. Vigil, D. Sun, M.W. Bates, T. Loman, E.A. Murphy, S.M. Barbon, J.-A. Song, B. Yu, G.H. **Fredrickson**, A.K. Whittaker, C.J. **Hawker**, C.M. **Bates**, Emergence of hexagonally close-packed spheres in linear block copolymer melts, *J. Am. Chem. Soc.* **143** (2021) 14106–14114. DOI: 10.1021/jacs.1c03647

**b. Partial MRSEC Support that Acknowledge the MRSEC Award DMR-1720256 [15]**

24. M. Ciavarella, G. Cricri, R. **McMeeking**, A comparison of crack propagation theories in viscoelastic materials, *Theor. Appl. Fract. Mech.* **116** (2021) 103113.  
DOI: 10.1016/j.tafmec.2021.103113
25. M. Ciavarella, A. Papangelo, R. **McMeeking**, Crack propagation at the interface between viscoelastic and elastic materials, *Eng. Fract. Mech.* **257** (2021) 108009.  
DOI: 10.1016/j.engfracmech.2021.108009
26. N. Cohen, C.D. Eisenbach, Humidity-driven supercontraction and twist in spider silk, *Phys. Rev. Lett.* **128** (2022) 098101. DOI: 10.1103/PhysRevLett.128.098101
27. V. Deshpande, A. DeSimone, R. **McMeeking**, P. Recho, Chemo-mechanical model of a cell as a stochastic active gel, *J. Mech. Phys. Solids* **151** (2021) 104381.  
DOI: 10.1016/j.jmps.2021.104381
28. N.D. Dolinski, E.B. Callaway, C.S. Sample, L.F. Gockowski, R. Chavez, Z.A. Page, F. Eisenreich, S. Hecht, M.T. **Valentine**, F.W. Zok, C.J. **Hawker**, Tough multimaterial interfaces through wavelength-selective 3D printing, *ACS Appl. Mater. Interfaces* **13** (2021) 22065–22072. DOI: 10.1021/acsami.1c06062
29. R. Goh, S.P.O. Danielsen, E. Schaible, R.M. **McMeeking**, J.H. **Waite**, Nanolatticed architecture mitigates damage in shark egg cases, *Nano Lett.* **21** (2021) 8080–8085.  
DOI: 10.1021/acs.nanolett.1c02439

30. M. Gu, Y. Luo, Y. He, M.E. **Helgeson**, M.T. **Valentine**, Uncertainty quantification and estimation in differential dynamic microscopy, *Phys. Rev. E* **104** (2021) 034610. DOI: 10.1103/PhysRevE.104.034610
31. M. Levin, M.T. **Valentine**, N. Cohen, Tuning the response of fluid filled hydrogel core-shell structures, *J. Mech. Behav. Biomed. Mater.* **120** (2021) 104605. DOI: 10.1016/j.jmbbm.2021.104605
32. E.O. McGhee, A.L. Chau, M.C. Cavanaugh, J.G. Rosa, C.L.G. Davidson IV, J. Kim, J.M. Urueña, B.S. Sumerlin, A.A. **Pitenis**, W.G. Sawyer, Amphiphilic gel lubrication and the solvophilic transition, *Biotribology* **26** (2021) 100170. DOI: 10.1016/j.biотri.2021.100170
33. S. Najafi, Y. Lin, A.P. Longhini, X. Zhang, K.T. Delaney, K.S. Kosik, G.H. **Fredrickson**, J-E. **Shea**, S. Han, Liquid–liquid phase separation of Tau by self and complex coacervation, *Protein Sci.* **30** (2021) 1393–1407. DOI: 10.1002/pro.4101
34. S.E. Seo, Y. Kwon, N.D. Dolinski, C.S. Sample, J.L. Self, C.M. **Bates**, M.T. **Valentine**, C.J. **Hawker**, Three-dimensional photochemical printing of thermally activated polymer foams, *ACS Appl. Polym. Mater.* **3** (2021) 4984–4991. DOI: 10.1021/acsapm.1c00726
35. J-E. **Shea**, R.B. Best, J. Mittal, Physics-based computational and theoretical approaches to intrinsically disordered proteins, *Curr. Opin. Struct. Biol.* **67** (2021) 219–225. DOI: 10.1016/j.sbi.2020.12.012
36. M.M. Sroda, J. Lee, Y. Kwon, F. Stricker, M. Park, M.T. **Valentine**, J. **Read de Alaniz**, Role of material composition in photothermal actuation of DASA-based polymers, *ACS Appl. Polym. Mater.* **4** (2022) 141–149. DOI: 10.1021/acsapm.1c01108
37. B.G.P. van Ravenstein, R.B. Zerdan, C.J. **Hawker**, M.E. **Helgeson**, Role of architecture on thermorheological properties of poly(alkyl methacrylate)-based polymers, *Macromolecules* **54** (2021) 5473–5483. DOI: 10.1021/acs.macromol.1c00149
38. X. Zhu, C. Wei, H. Chen, C. Zhang, H. Peng, D. Wang, J. Yuan, J.H. **Waite**, Q. Zhao, A cation-methylene-phenyl sequence encodes programmable poly(ionic liquid) coacervation and robust underwater adhesion, *Adv. Funct. Mater.* **32** (2021) 2105464. DOI: 10.1002/adfm.202105464

## SEED [9]

### a. Primary MRSEC Support that Acknowledge the MRSEC Award DMR-1720256 [3]

39. B.B. Haidet, L. Nordin, A.J. Muhowski, K.D. Vallejo, E.T. Hughes, J. Meyer, P.J. Simmonds, D. Wasserman, K. Mukherjee, Interface structure and luminescence properties of epitaxial PbSe films on InAs(111)A, *J. Vac. Sci. Tech. A* **39** (2021) 023404. DOI: 10.1116/6.0000774
40. E.T. Hughes, B.B. Haidet, B. Bonef, W. Cai, K. Mukherjee, Pipe-diffusion-enriched dislocations and interfaces in SnSe/PbSe heterostructures, *Phys. Rev. Mater.* **5** (2021) 73402. DOI: 10.1103/PhysRevMaterials.5.073402
41. M.E. Turiansky, C.G. Van de Walle, Impact of dangling bonds on properties of h-BN, *2D Mater.* **8** (2021) 024002. DOI: 10.1088/2053-1583/abe4bb  
(Published 25 February 2021. This paper was missed when compiling last year's report.)

**b. Partial MRSEC Support that Acknowledge the MRSEC Award DMR-1720256 [6]**

42. J. Meyer, A.J. Muhowski, L. Nordin, E. Hughes, B. Haidet, D. Wasserman, K. Mukherjee, Bright mid-infrared photoluminescence from high dislocation density epitaxial PbSe films on GaAs, *APL Mater.* **9** (2021) 111112. DOI: 10.1063/5.0070555
43. J. Orenstein, J.E. Moore, T. Morimoto, D.H. Torchinsky, J.W. Harter, D. Hsieh, Topology and symmetry of quantum materials via nonlinear optical responses, *Annu. Rev. Condens. Matter Phys.* **12** (2021) 247–272. DOI: 10.1146/annurev-conmatphys-031218-013712
44. L. Razinkovas, M.W. Doherty, N.B. Manson, C.G. Van de Walle, A. Alkauskas, Vibrational and vibronic structure of isolated point defects: The nitrogen-vacancy center in diamond, *Phys. Rev. B* **104** (2021) 045303. DOI: 10.1103/PhysRevB.104.045303
45. M. Romanova, V. Vlček, Stochastic many-body calculations of moiré states in twisted bilayer graphene at high pressures, *npj Comput. Mater.* **8** (2022) Article number: 11. DOI: 10.1038/s41524-022-00697-8
46. J-X. Shen, M.E. Turiansky, D. Wickramaratne, C.G. Van de Walle, Thermodynamics of boron incorporation in BGaN, *Phys. Rev. Mater.* **5** (2021) L030401. DOI: 10.1103/PhysRevMaterials.5.L030401
47. H. Zhao, H. Li, L. Dong, B. Xu, J. Schneeloch, R. Zhong, M. Fang, G. Gu, J. Harter, S.D. Wilson, Z. Wang, I. Zeljkovic, Nematic transition and nanoscale suppression of superconductivity in Fe(Te,Se), *Nat. Phys.* **17** (2021) 903–908. DOI: 10.1038/s41567-021-01254-8

**iSUPERSEED [3]**

**a. Primary MRSEC Support that Acknowledge the MRSEC Award DMR-1720256 [0]**

None

**b. Partial MRSEC Support that Acknowledge the MRSEC Award DMR-1720256 [3]**

48. M.J. Bowick, N. Fakhri, M.C. Marchetti, S. Ramaswamy, Symmetry, thermodynamics, and topology in active matter, *Phys. Rev. X* **12** (2022) 010201. DOI: 10.1103/PhysRevX.12.010501
49. P.Z. Hanakata, S.S. Bhabesh, M.J. Bowick, D.R. Nelson, D. Yllanes, Thermal buckling and symmetry breaking in thin ribbons under compression, *Extreme Mech. Lett.* **44** (2021) 101270. DOI: 10.1016/j.eml.2021.101270
50. F. Vafa, M.J. Bowick, B.I. Shraiman, M.C. Marchetti, Fluctuations can induce local nematic order and extensile stress in monolayers of motile cells, *Soft Matter* **17** (2021) 3068–3073. DOI: 10.1039/D0SM02027C

## SHARED FACILITIES [191]

51. M. Abdelghany, A.A. Farid, M.E. Rasekh, U. Madhow, M.J.W. Rodwell, A design framework for all-digital mmWave massive MIMO with per-antenna nonlinearities, *IEEE Trans. Wireless Commun.* **20** (2021) 5689–5701. DOI: 10.1109/TWC.2021.3069378
52. C. Albrecht, A. Kumar, S. Xu, A. Hunter, I.J. Beyerlein, Asymmetric equilibrium core structures of pyramidal-II  $\langle c+a \rangle$  dislocations in ten hexagonal-close-packed metals, *Phys. Rev. Mater.* **5** (2021) 043602. DOI: 10.1103/PhysRevMaterials.5.043602
53. A.S. Almogbel, C.J. Zollner, B.K. Saifaddin, M. Iza, J. Wang, Y. Yao, M. Wang, H. Foronda, I. Prozheev, F. Tuomisto, A. Albadri, S. Nakamura, S.P. DenBaars, J.S. Speck, Growth of highly conductive Al-rich AlGaN:Si with low group-III vacancy concentration, *AIP Adv.* **11** (2021) 095119. DOI: 10.1063/5.0066652
54. M.S. Andrei, J.S.J. Hsu, A Bayesian approach for large asset allocation, *Int. J. Stat. Prob.* **10** (2021) 58–68. DOI: 10.5539/ijsp.v10n1p58  
(Published January 2021. This paper was missed when compiling last year's report.)
55. S. Antoine, Z. Geng, E.S. Zofchak, M. Chwatko, G.H. **Fredrickson**, V. Ganesan, C.J. **Hawker**, N.A. Lynd, R.A. **Segalman**, Non-intuitive trends in Flory–Huggins interaction parameters in polyether-based polymers, *Macromolecules* **54** (2021) 6670–6677. DOI: 10.1021/acs.macromol.1c00134
56. A. Apigo, R. Oono, Plant abundance, but not plant evolutionary history, shapes patterns of host specificity in foliar fungal endophytes, *Ecosphere* **13** (2022) e03879. DOI: 10.1002/ecs2.3879
57. S.W. Baek, M.B. Preefer, M. Saber, K. Zhai, M. Frajnkovič, Y. Zhou, B.S. Dunn, A. **Van der Ven**, R. **Seshadri**, L. Pilon, Potentiometric entropy and *operando* calorimetric measurements reveal fast charging mechanisms in PNb<sub>9</sub>O<sub>25</sub>, *J. Power Sources* **520** (2022) 230776. DOI: 10.1016/j.jpowsour.2021.230776
58. S.W. Baek, K.E. Wyckoff, D.M. Butts, J. Bienz, A. Likitchatchawankun, M.B. Preefer, M. Frajnkovič, B.S. Dunn, R. **Seshadri**, L. Pilon, *Operando* calorimetry informs the origin of rapid rate performance in microwave-prepared TiNb<sub>2</sub>O<sub>7</sub> electrodes, *J. Power Sources* **490** (2021) 229537. DOI: 10.1016/j.jpowsour.2021.229537
59. G.H. Balbus, J. Kappacher, D.J. Sprouster, F. Wang, J. Shin, Y.M. Eggeler, T.J. Rupert, J.R. Trelewicz, D. Kiener, V. Maier-Kiener, D.S. **Gianola**, Disordered interfaces enable high temperature thermal stability and strength in a nanocrystalline aluminum alloy, *Acta Mater.* **215** (2021) 116973. DOI: 10.1016/j.actamat.2021.116973
60. J.A. Barrett, Z. Li, J.V. Garcia, E. Wein, D. Zheng, C. Hunt, L. Ngo, L. Sepunaru, A.V. Iretskii, P.C. Ford, Redox-mediated carbon monoxide release from a manganese carbonyl—implications for physiological CO delivery by CO releasing moieties, *R.Soc. Open Sci.* **8** (2021) 211022. DOI: 10.1098/rsos.211022
61. N.H. Bashian, M. Zuba, A. Irshad, S.M. Becwar, J. Vinckevisciute, W. Rahim, K.J. Griffith, E.T. McClure, J.K. Papp, B.D. McCloskey, D.O. Scanlon, B.F. **Chmelka**, A. **Van der Ven**, S.R. Narayan, L.F. J. Piper, B.C. Melot, Electrochemical oxidative fluorination of an oxide perovskite, *Chem. Mater.* **33** (2021) 5757–5768. DOI: 10.1021/acs.chemmater.1c01594

62. A.V. Bayles, J.M. Fisher, C.S. Valentine, A. Nowbahar, M.E. **Helgeson**, T.M. Squires, Hydrogen bonding strength determines water diffusivity in polymer ionogels, *J. Phys. Chem. B* **125** (2021) 5408–5419. DOI: 10.1021/acs.jpcb.1c01460
63. M.M. Bordelon, X. Wang, D.M. Pajerowski, A. Banerjee, M. Sherwin, C.M. Brown, M.S. Eldeeb, T. Petersen, L. Hozoi, U.K. Roßler, M. Mourigal, S.D. **Wilson**, Magnetic properties and signatures of moment ordering in the triangular lattice antiferromagnet KCeO<sub>2</sub>, *Phys. Rev. B* **104** (2021) 094421. DOI: 10.1103/PhysRevB.104.094421
64. C. Braun, C. Nusbaum, P. Rupert, Labor market dynamics and the migration behavior of married couples, *Rev. Econom. Dynamics* **42** (2021) 239–263. DOI: 10.1016/j.red.2020.11.001
65. L.K. Bryngemark, D. Cameron, V. Dutta, T. Eichlersmith, B. Konya, O. Moreno, G. Mullier, F. Paganelli, R. Pöttgen, F. Rogers, A. Salnikov, P. Weakliem, Building a distributed computing system for LDMX: Challenges of creating and operating a lightweight e-infrastructure for small-to-medium size accelerator experiments, *EPJ Web of Conferences* **251** (2021) 02038. DOI: 10.1051/epjconf/202125102038
66. Z. Cai, H. Ji, Y. Ha, J. Liu, D-H. Kwon, Y. Zhang, A. Urban, E.E. Foley, R. Giovine, H. Kim, Z. Lun, T-Y. Huang, G. Zeng, Y. Chen, J. Wang, B.D. McCloskey, M. Balasubramanian, R.J. **Clément**, W. Yang, G. Ceder, Realizing continuous cation order-to-disorder tuning in a class of high-energy spinel-type Li-ion cathodes, *Matter* **4** (2021) 3897–3916. DOI: 10.1016/j.matt.2021.10.013
67. K.Y. Camsari, M.M. Torunbalci, W.A. Borders, H. Ohno, S. Fukami, Double-free-layer magnetic tunnel junctions for probabilistic bits, *Phys. Rev. Appl.* **15** (2021) 044049. DOI: 10.1103/PhysRevApplied.15.044049
68. P. Chan, S.P. DenBaars, S. Nakamura, Growth of highly relaxed InGaN pseudo-substrates over full 2-in. wafers, *Appl. Phys. Lett.* **119** (2021) 131106. DOI: 10.1063/5.0064755
69. P. Chan, C.E. Reilly, S. Keller, S.P. DenBaars, S. Nakamura, Growth by MOCVD and photoluminescence of semipolar (2021)InN quantum dashes, *J. Cryst. Growth* **563** (2021) 126093. DOI: 10.1016/j.jcrysgro.2021.126093
70. P. Chan, V. Rienzi, N. Lim, H-M. Chang, M. Gordon, S.P. DenBaars, S. Nakamura, Demonstration of relaxed InGaN-based red LEDs grown with high active region temperature, *Appl. Phys. Express* **14** (2021) 101002. DOI: 10.35848/1882-0786/ac251d
71. M.A. Charpagne, J.M. Hestroffer, A.T. Polonsky, M.P. Echlin, D. Texier, V. Valle, I.J. Beyerlein, T.M. **Pollock**, J.C. Stinville, Slip localization in Inconel 718: A three-dimensional and statistical perspective, *Acta Mater.* **215** (2021) 117037. DOI: 10.1016/j.actamat.2021.117037
72. M.A. Charpagne, J.C. Stinville, A.T. Polonsky, M.P. Echlin, T.M. **Pollock**, A multi-modal data merging framework for correlative investigation of strain localization in three dimensions, *J. Minerals, Metals & Mater. Soc.* **73** (2021) 3263–3271. DOI: 10.1007/s11837-021-04894-6
73. S. Chatterjee, F. Crasto de Lima, J.A. Logan, Y. Fang, H. Inbar, A. Goswami, C. Dempsey, J. Dong, S. Khalid, T. Brown-Heft, Y-H. Chang, T. Guo, D.J. Pennachio, N. Wilson, S. Chikara, A. Suslov, A.V. Fedorov, D. Read, J. Cano, A. Janotti, C.J. Palmstrøm, Identifying the fingerprints of topological states by tuning magnetoresistance in a

- semimetal: The case of topological half-Heusler  $\text{Pt}_{1-x}\text{Au}_x\text{LuSb}$ , *Phys. Rev. Mater.* **5** (2021) 124207. DOI: 10.1103/PhysRevMaterials.5.124207
74. S. Chatterjee, S. Khalid, H.S. Inbar, A. Goswami, T. Guo, Y-H. Chang, E. Young, A.V. Fedorov, D. Read, A. Janotti, C.J. Palmstrøm, Controlling magnetoresistance by tuning semimetallicity through dimensional confinement and heteroepitaxy, *Sci. Adv.* **7** (2021) eabe8971. DOI: 10.1126/sciadv.abe8971
75. Z. Chen, Z. Qu, L. Liu, Y. Ding, Y. Xie, 'Efficient tensor core-based GPU kernels for structured sparsity under reduced precision', *SC '21: Proc. of the Int. Conference for High Performance Computing, Networking, Storage and Analysis*, November 14–19, 2021, St. Louis, Missouri. Article No.: 78 (2021) 1–14. DOI: 10.1145/3458817.3476182
76. Z. Chen, D. Wan, M.J. **Bowick**, Spontaneous tilt of single-clamped thermal elastic sheets, *Phys. Rev. Lett.* **128** (2022) 028006. DOI: 10.1103/PhysRevLett.128.028006
77. X. Cheng, T. Li, K. Gutman, L. Zhang, Chiral bifunctional phosphine ligand-enabled cooperative Cu catalysis: Formation of chiral  $\alpha,\beta$ -Butenolides via highly enantioselective  $\gamma$ -protonation, *J. Am. Chem. Soc.* **143** (2021) 10876–10881. DOI: 10.1021/jacs.1c05781
78. A. Chialastri, C. Wangsanuwat, S.S. Dey, Integrated single-cell sequencing of 5-hydroxymethylcytosine and genomic DNA using scH&G-seq, *STAR Protocols* **2** (2021) 101016. DOI: 10.1016/j.xpro.2021.101016
79. C. Choi, J.L. Self, Y. Okayama, A.E. Levi, M. Gerst, J.C. Speros, C.J. **Hawker**, J. **Read de Alaniz**, C.M. **Bates**, Light-mediated synthesis and reprocessing of dynamic bottlebrush elastomers under ambient conditions, *J. Am. Chem. Soc.* **143** (2021) 9866–9871. DOI: 10.1021/jacs.1c03686
80. J. Chung, P. Hertler, K.W. Plaxco, L. Sepunaru, Catalytic interruption mitigates edge effects in the characterization of heterogeneous, insulating nanoparticles, *J. Am. Chem. Soc.* **143** (2021) 18888–18898. DOI: 10.1021/jacs.1c04971
81. D.B. Culver, R.W. Dorn, A. Venkatesh, J. Meeprasert, A.J. Rossini, E.A. Pidko, A.S. Lipton, G.R. Lief, M.P. Conley, Active sites in a heterogeneous organometallic catalyst for the polymerization of ethylene, *ACS Cent. Sci.* **7** (2021) 1225–1231. DOI: 10.1021/acscentsci.1c00466
82. S.P.O. Danielsen, C.R. Bridges, R.A. **Segalman**, Chain stiffness of donor–acceptor conjugated polymers in solution, *Macromolecules* **55** (2022) 437–449. DOI: 10.1021/acs.macromol.1c02229
83. P.R. Dawson, M.P. Miller, T.M. **Pollock**, J. Wendorf, L.H. Mills, J.C. Stinville, M.A. Charpagne, M.P. Echlin, Mechanical metrics of virtual polycrystals (MechMet), *Integr. Mater. Manuf. Innovation* **10** (2021) 265–285. DOI: 10.1007/s40192-021-00206-7
84. G.D. Degen, P. Delparastan, B.D.B. Tiu, P.B. Messersmith, Surface force measurements of mussel-inspired pressure-sensitive adhesives, *ACS Appl. Mater. Interfaces* **14** (2022) 6212–6220. DOI: 10.1021/acsami.1c22295
85. L. Detering, A. Abdilla, H.P. Luehmann, J.W. Williams, L-H. Huang, D. Sultan, A. Elvington, G. S. Heo, P.K. Woodard, R.J. Gropler, G.J. Randolph, C.J. **Hawker**, Y. Liu, CC chemokine receptor 5 targeted nanoparticles imaging the progression and regression of atherosclerosis using positron emission tomography/computed tomography, *Mol. Pharmaceutics* **18** (2021) 1386–1396. DOI: 10.1021/acs.molpharmaceut.0c01183

86. Z. Ding, C. Zhu, M. De Graef, Determining crystallographic orientation via hybrid convolutional neural network, *Mater. Charact.* **178** (2021) 111213.  
DOI: 10.1016/j.matchar.2021.111213
87. M.P. Echlin, M. Kasemer, K. Chatterjee, D. Boyce, J. C. Stinville, P.G. Callahan, E. Wielewski, J-S. Park, J.C. Williams, R.M. Suter, T.M. **Pollock**, M.P. Miller, P.R. Dawson, Microstructure-based estimation of strength and ductility distributions for  $\alpha+\beta$  titanium alloys, *Metall. Mater. Trans. A* **52** (2021) 2411–2434. DOI: 10.1007/s11661-021-06233-5
88. R. Egan, A. Guittet, F. Temprano-Coleto, T. Isaac, F.J. Peaudecerf, J.R. Landel, P. Luzzatto-Fegiz, C. Burstedde, F. Gibou, Direct numerical simulation of incompressible flows on parallel Octree grids, *J. Comput. Phys.* **428** (2021) 110084.  
DOI: 10.1016/j.jcp.2020.110084
89. B. Emery, A. Kirincich, L. Washburn, Direction finding and likelihood ratio detection for oceanographic HF radars, *J. Atmos. Oceanic Technol.* **39** (2022) 223–235.  
DOI: 10.1175/JTECH-D-21-0110.1
90. K.K. Ewert, P. Scodeller, L. Simón-Gracia, V.M. Steffes, E.A. Wonder, T. Teesalu, C.R. Safinya, Cationic liposomes as vectors for nucleic acid and hydrophobic drug therapeutics, *Pharmaceutics* **13** (2021) 1365. DOI: 10.3390/pharmaceutics13091365
91. L.T.W. Fey, S. Xu, Y. Su, A. Hunter, I.J. Beyerlein, Transitions in the morphology and critical stresses of gliding dislocations in multiprincipal element alloys, *Phys. Rev. Mater.* **6** (2022) 013605. DOI: 10.1103/PhysRevMaterials.6.013605
92. J. Finzel, P. Christopher, Dynamic Pt coordination in dilute AgPt alloy nanoparticle catalysts under reactive environments, *Top. Catal.* (2022).  
DOI: 10.1007/s11244-021-01545-7
93. E.E. Foley, A. Wong, R.C. Vincent, A. Manche, A. Zaveri, E. Gonzalez-Correa, G. Ménard, R.J. **Clément**, Probing reaction processes and reversibility in Earth-abundant Na<sub>3</sub>FeF<sub>6</sub> for Na-ion batteries, *Phys. Chem. Chem. Phys.* **23** (2021) 20052. DOI: 10.1039/d1cp02763h
94. L. Galletti, A. Rashidi, D.A. Kealhofer, M. Goyal, B. Guo, Y. Li, C. Shang, J.E. Bowers, S. Stemmer, Quantum Hall effect of the topological insulator state of cadmium arsenide in Corbino geometry, *Appl. Phys. Lett.* **118** (2021) 261901. DOI: 10.1063/5.0056357
95. S. Ghosh, N. Barman, E. Gonzalez-Correa, M. Mazumder, A. Zaveri, R. Giovine, A. Manche, S.K. Pati, R.J. **Clément**, P. Senguttuvan, Elucidating the impact of Mg substitution on the properties of NASICON-Na<sub>3+y</sub>V<sub>2-y</sub>Mg<sub>y</sub>(PO<sub>4</sub>)<sub>3</sub> cathodes, *Adv. Funct. Mater.* **31** (2021) 2105463. DOI: 10.1002/adfm.202105463
96. J.G. Goiri, A. **Van der Ven**, MultiShifter: Software to generate structural models of extended two-dimensional defects in 3D and 2D crystals, *Comput. Mater. Sci.* **191** (2021) 110310. DOI: 10.1016/j.commatsci.2021.110310
97. A. Goswami, B. Markman, S.T. Šuran Brunelli, S. Chatterjee, J. Klamkin, M. Rodwell, C.J. Palmstrøm, Confined lateral epitaxial overgrowth of InGaAs: Mechanisms and electronic properties, *J. Appl. Phys.* **130** (2021) 085302. DOI: 10.1063/5.0050802
98. N.S.H. Gunda, C.G. Levi, A. **Van der Ven**, Investigating the electronic origins of the repulsion between substitutional and interstitial solutes in hcp Ti, *Phys. Rev. Mater.* **5** (2021) 073604. DOI: 10.1103/PhysRevMaterials.5.073604

99. R.T. Hannagan, G. Giannakakis, R. Réocreux, J. Schumann, J. Finzel, Y. Wang, A. Michaelides, P. Deshlahra, P. Christopher, M. Flytzani-Stephanopoulos, M. Stamatakis, E.C.H. Sykes, First-principles design of a single-atom–alloypropane dehydrogenation catalyst, *Science* **372** (2021) 1444–1447. DOI: 10.1126/science.abg8389
100. K.G. Hanson, C-H. Lin, M.M. Abu-Omar, Crosslinking of renewable polyesters with epoxides to form bio-based epoxy thermosets, *Polymer* **238** (2022) 124363. DOI: 10.1016/j.polymer.2021.124363
101. K.G. Hanson, C-H. Lin, M.M. Abu-Omar, Preparation and properties of renewable polyesters based on lignin-derived bisphenol, *Polymer* **233** (2021) 124202. DOI: 10.1016/j.polymer.2021.124202
102. K. Hejazi, X. Chen, L. Balents, Hybrid Wannier Chern bands in magic angle twisted bilayer graphene and the quantized anomalous Hall effect, *Phys. Rev. Res.* **3** (2021) 013242. DOI: 10.1103/PhysRevResearch.3.013242
103. A.J. Hoffman, C. Asokan, N. Gadinas, P. Kravchenko, A. Getsoian, P. Christopher, D. Hibbits, Theoretical and experimental characterization of adsorbed CO and NO on  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>-supported Rh nanoparticles, *J. Phys. Chem. C* **125** (2021) 19733–19755. DOI: 10.1021/acs.jpcc.1c05160
104. C.S. Holgate, G.G.E. Seward, A.R. Ericks, D.L. Poerschke, C.G. Levi, Dissolution and diffusion kinetics of yttria-stabilized zirconia into molten silicates, *J. Eur. Ceram. Soc.* **41** (2021) 1984–1994. DOI: 10.1016/j.jeurceramsoc.2020.10.056
105. C.S. Holgate, Y.L. Yang, C.G. Levi, Reactive crystallization in HfO<sub>2</sub> exposed to molten silicates, *J. Eur. Ceram. Soc.* **41** (2021) 5686–5695. DOI: 10.1016/j.jeurceramsoc.2021.03.025
106. E. Hughes, B. Haidet, B. Bonef, J. Selvidge, C. Shang, J. Norman, J. Bowers, K. Mukherjee, Advances in heteroepitaxial integration of III-V and IV-VI semiconductors with electron channeling contrast imaging, *Microsc. Microanal.* **27** (2021) 908. (Suppl 1). DOI: 10.1017/S1431927621003494
107. D.K. Jangid, N.R. Brodnik, A. Khan, M.G. Goebel, M.P. Echlin, T.M. Pollock, S.H. Daly, B.S. Manjunath, 3D grain shape generation in polycrystals using generative adversarial networks, *Integr. Mater. Manuf. Innovation* **11** (2022) 71–84. DOI: 10.1007/s40192-021-00244-1
108. H. Jeong, N.G. Combs, S. Munyan, A. Rashidi, S. Stemmer, Reducing surface depletion of superconducting SrTiO<sub>3</sub> films with EuTiO<sub>3</sub> capping layers, *Appl. Phys. Lett.* **119** (2021) 162601. DOI: 10.1063/5.0067681
109. W-R. Jian, Y. Su, S. Xu, W. Ji, I.J. Beyerlein, Effect of interface structure on dislocation glide behavior in nanolaminates, *J. Mater. Res.* **36** (2021) 2802–2815. DOI: 10.1557/s43578-021-00261-y
110. W-R. Jian, L. Wang, W. Bi, S. Xu, I.J. Beyerlein, Role of local chemical fluctuations in the melting of medium entropy alloy CoCrNi, *Appl. Phys. Lett.* **119** (2021) 121904. DOI: 10.1063/5.0064299
111. W-R. Jian, S. Xu, I.J. Beyerlein, On the significance of model design in atomistic calculations of the Peierls stress in Nb, *Comput. Mater. Sci.* **188** (2021) 110150. DOI: 10.1016/j.commatsci.2020.110150  
(Published 15 February 2021. This paper was missed when compiling last year's report.)

112. Y-X. Jiang, J-X. Yin, M. M. Denner, N. Shumiya, B.R. Ortiz, G. Xu, Z. Guguchia, J. He, Md S. Hossain, X. Liu, J. Ruff, L. Kautzsch, S.S. Zhang, G. Chang, I. Belopolski, Q. Zhang, T.A. Cochran, D. Multer, M. Litskevich, Z-J. Cheng, X.P. Yang, Z. Wang, R. Thomale, T. Neupert, S.D. **Wilson**, M.Z. Hasan, Unconventional chiral charge order in kagome superconductor  $KV_3Sb_5$ , *Nat. Mater.* **20** (2021) 1353–1357. DOI: 10.1038/s41563-021-01034-y
113. S. Jiao, A. DeStefano, J.I. Monroe, M. Barry, N. Sherck, T. Casey, R.A. **Segalman**, S. Han, M.S. Shell, Quantifying polypeptoid conformational landscapes through integrated experiment and simulation, *Macromolecules* **54** (2021) 5011–5021. DOI: 10.1021/acs.macromol.1c00550
114. J.M. Johnson, H-L. Huang, M. Wang, S. Mu, J.B. Varley, A.F.M.A.U. Bhuiyan, Z. Feng, N.K. Kalarickal, S. Rajan, H. Zhao, C.G. Van de Walle, J. Hwang, Atomic scale investigation of aluminum incorporation, defects, and phase stability in  $\beta$ - $(Al_xGa_{1-x})_2O_3$  films, *APL Mater.* **9** (2021) 051103. DOI: 10.1063/5.0039769
115. J.L. Kaufman, A. **Van der Ven**, Antiphase boundary migration as a diffusion mechanism in a P3 sodium layered oxide, *Phys. Rev. Mater.* **5** (2021) 055401. DOI: 10.1103/PhysRevMaterials.5.055401
116. J.L. Kaufman, A. **Van der Ven**, Cation diffusion facilitated by antiphase boundaries in layered intercalation compounds, *Chem. Mater.* **34** (2022) 1889–1896. DOI: 10.1021/acs.chemmater.1c04152
117. D.A. Kealhofer, M. Goyal, T.N. Pardue, S. Stemmer, Thickness-independent transport in thin (001)-oriented cadmium arsenide films, *Phys. Rev. B* **104** (2021) 035435. DOI: 10.1103/PhysRevB.104.035435
118. S. Keller, S.S. Pasayat, C. Gupta, S.P. DenBaars, S. Nakamura, U.K. Mishra, Patterned III-nitrides on porous GaN: Extending elastic relaxation from the nano- to the micrometer scale, *Phys. Status Solidi RRL* **15** (2021) 2100234. DOI: 10.1002/pssr.202100234
119. R.M. Kennard, C.J. Dahlman, J. Chung, B.L. Cotts, A.A. Mikhailovsky, L. Mao, R.A. DeCrescent, K.H. Stone, N.R. Venkatesan, Y. Mohtashami, S. Assadi, A. Salleo, J.A. Schuller, R. **Seshadri**, M.L. **Chabiny**, Growth-controlled broad emission in phase-pure two-dimensional hybrid perovskite films, *Chem. Mater.* **33** (2021) 7290–7300. DOI: 10.1021/acs.chemmater.1c01641
120. E.M. Kenney, B.R. Ortiz, C. Wang, S.D. **Wilson**, M.J. Graf, Absence of local moments in the kagome metal  $KV_3Sb_5$  as determined by muon spin spectroscopy, *J. Phys.: Condens. Matter* **33** (2021) 235801. DOI: 10.1088/1361-648X/abe8f9
121. A. Keselman, L. Nie, E. Berg, Scrambling and Lyapunov exponent in spatially extended systems, *Phys. Rev. B* **103** (2021) L12111. DOI: 10.1103/PhysRevB.103.L12111
122. V. Khanna, J. Anwar, D. Frenkel, M.F. Doherty, B. Peters, Free energies of crystals computed using Einstein crystal with fixed center of mass and differing spring constants, *J. Chem. Phys.* **154** (2021) 164509. DOI: 10.1063/5.0044833
123. A. Khindanov, J. Alicea, P. Lee, W.S. Cole, A.E. Antipov, Topological superconductivity in nanowires proximate to a diffusive superconductor–magnetic-insulator bilayer, *Phys. Rev. B* **103** (2021) 134506. DOI: 10.1103/PhysRevB.103.134506
124. S. Kim, M. Pochitaloff, G.A. Stooke-Vaughan, O. Campàs, Embryonic tissues as active foams, *Nat. Phys.* **17** (2021) 859–866. DOI: 10.1038/s41567-021-01215-1

125. S.K. Kolli, A.R. Natarajan, A. **Van der Ven**, Six new transformation pathways connecting simple crystal structures and common intermetallic crystal structures, *Acta Mater.* **221** (2021) 117429. DOI: 10.1016/j.actamat.2021.117429
126. K. Krishnaswamy, A. Janotti, L. Bjaalie, C.G. Van de Walle, Surprising stability of polar (001) surfaces of the Mott insulator  $\text{GdTiO}_3$ , *J. Vac. Sci. Technol., A* **39** (2021) 063220. DOI: 10.1116/6.0001313
127. P. Kumar, J.B. Rawlings, S.J. Wright, Industrial, large-scale model predictive control with structured neural networks, *Comput. Chem. Eng.* **150** (2021) 107291. DOI: 10.1016/j.compchemeng.2021.107291
128. L.A. Larios-Cardenas, F. Gibou, A deep learning approach for the computation of curvature in the level-set method, *SIAM J. Sci. Comput.* **43** (2021) A1754–A1779. DOI: 10.1137/20M1316755
129. M.L. Le, D. Rawlings, S.P.O. Danielsen, R.M. Kennard, M.L. **Chabiny**, R.A. **Segalman**, Aqueous formulation of concentrated semiconductive fluid using polyelectrolyte coacervation, *ACS Macro Lett.* **10** (2021) 1008–1014. DOI: 10.1021/acsmacrolett.1c00354
130. S. Lei, S.M.L. Teicher, A. Topp, K. Cai, J. Lin, G. Cheng, T.H. Salters, F. Rodolakis, J.L. McChesney, S. Lapidus, N. Yao, M. Krivenkov, D. Marchenko, A. Varykhalov, C.R. Ast, R. Car, J. Cano, M.G. Vergniory, N.P. Ong, L.M. Schoop, Band engineering of Dirac semimetals using charge density waves, *Adv. Mater.* **33** (2021) 2101591. DOI: 10.1002/adma.202101591
131. B.D.A. Levin, Direct detectors and their applications in electron microscopy for materials science, *J. Phys.: Mater.* **4** (2021) 042005. DOI: 10.1088/2515-7639/ac0ff9
132. W. Li, K.T. Delaney, G.H. **Fredrickson**, Self-consistent field theory study of polymer-mediated colloidal interactions in solution: Depletion effects and induced forces, *J. Chem. Phys.* **155** (2021) 154903. DOI: 10.1063/5.0065742
133. Y. Li, X. Chen, A.W.W. Ludwig, M.P.A. Fisher, Conformal invariance and quantum nonlocality in critical hybrid circuits, *Phys. Rev. B* **104** (2021) 104305. DOI: 10.1103/PhysRevB.104.104305
134. Y. Li, M.P.A. Fisher, Statistical mechanics of quantum error correcting codes, *Phys. Rev. B* **103** (2021) 104306. DOI: 10.1103/PhysRevB.103.104306
135. C. Liu, P. Zhang, X. Chen, Non-unitary dynamics of Sachdev-Ye-Kitaev chain, *SciPost Phys.* **10** (2021) 048. DOI: 10.21468/SciPostPhys.10.2.048  
(Published 23 February 2021. This paper was missed when compiling last year's report.)
136. L. Liu, J. Lin, Z. Qu, Y. Ding, Y. Xie, 'ENMC: Extreme near-memory classification via approximate screening', *MICRO'21: 54th Annual IEEE/ACM Intl. Symposium on Microarchitecture*, October 18–22, 2021, Virtual Event, Greece. ACM: New York, NY. Pages 1309–1322. DOI: 10.1145/3466752.3480090
137. J.L. Lyons, C.G. Van de Walle, Hole trapping at acceptor impurities and alloying elements in AlN, *Phys. Status Solidi RRL* **15** (2021) 2100218. DOI: 10.1002/pssr.202100218
138. G.G. Martirosyan, G.S. Hovhannisan, T.S. Kurtikyan, A.V. Iretskii, Matrix isolation infrared study of the interaction of dioxygen with chromium(II)tetraphenylporphyrin, *Inorg. Chim. Acta* **524** (2021) 120439. DOI: 10.1016/j.ica.2021.120439

139. C. Mejuto-Zaera, G. Weng, M. Romanova, S.J. Cotton, K.B. Whaley, N.M. Tubman, V. **Vlček**, Are multi-quasiparticle interactions important in molecular ionization? *J. Chem. Phys.* **154** (2021) 121101. DOI: 10.1063/5.0044060
140. A. Milekhin, Non-local reparametrization action in coupled Sachdev-Ye-Kitaev models, *J. High Energy Phys.* **2021** (2021) 114. DOI: 10.1007/JHEP12(2021)114
141. A. Miller-ter Kuile, A. Apigo, H.S. Young, Effects of consumer surface sterilization on diet DNA metabarcoding data of terrestrial invertebrates in natural environments and feeding trials, *Ecol. Evol.* **11** (2021) 12025–12034. DOI: 10.1002/ece3.7968
142. Y. Mohtashami, R. DeCrescent, L. Heki, P. Iyer, N. Butakov, M. Wong, A. Alhassan, W. Mitchell, S. Nakamura, S. DenBaars, J. Schuller, ‘Luminescent metalenses for focusing spontaneous emission’, *IEEE 2021 Fifteenth Intl. Congress on Artificial Materials for Novel Wave Phenomena (Metamaterials)*, September 20–25, 2021, New York City, NY. Pages X281–X283 (2021). DOI: 10.1109/Metamaterials52332.2021.9577175
143. Y. Mohtashami, R.A. DeCrescent, L.K. Heki, P.P. Iyer, N.A. Butakov, M.S. Wong, A. Alhassan, W.J. Mitchell, S. Nakamura, S.P. DenBaars, J.A. Schuller, Light-emitting metalenses and meta-axicons for focusing and beaming of spontaneous emission, *Nat. Commun.* **12** (2021) 3591. DOI: 10.1038/s41467-021-23433-0
144. H. Moon, R.P. Collanton, J.I. Monroe, T.M. Casey, M.S. Shell, S. Han, S.L. Scott, Evidence for entropically controlled interfacial hydration in mesoporous organosilicas, *J. Am. Chem. Soc.* **144** (2022) 1766–1777. DOI: 10.1021/jacs.1c11342
145. S. Mu, A.J. E. Rowberg, J. Leveillee, F. Giustino, C.G. Van de Walle, First-principles study of electron transport in ScN, *Phys. Rev. B* **104** (2021) 075118. DOI: 10.1103/PhysRevB.104.075118
146. K. Mukherjee, J. Selvidge, E. Hughes, J. Norman, C. Shang, R. Herrick, J. Bowers, Kinetically limited misfit dislocations formed during post-growth cooling in III–V lasers on silicon, *J. Phys. D: Appl. Phys.* **54** (2021) 494001. DOI: 10.1088/1361-6463/ac24c9
147. B.R. Ortiz, P.M. Sarte, E.M. Kenney, M.J. Graf, S.M.L. Teicher, R. **Seshadri**, S.D. **Wilson**, Superconductivity in the Z<sub>2</sub> kagome metal KV<sub>3</sub>Sb<sub>5</sub>, *Phys. Rev. Mater.* **5** (2021) 034801. DOI: 10.1103/PhysRevMaterials.5.034801
148. B.R. Ortiz, S.M.L. Teicher, L. Kautzsch, P.M. Sarte, N. Ratcliff, J. Harter, J.P.C. Ruff, R. **Seshadri**, S.D. **Wilson**, Fermi surface mapping and the nature of charge-density-wave order in the kagome superconductor CsV<sub>3</sub>Sb<sub>5</sub>, *Phys. Rev. X* **11** (2021) 041030. DOI: 10.1103/PhysRevX.11.041030
149. B. Oyang, Y-F. Jiang, O. Blaes, Investigating lack of accretion disc eccentricity growth in a global 3D MHD simulation of a superhump system, *Mon. Not. R. Astron. Soc.* **505** (2021) 1–17. DOI: 10.1093/mnras/stab1212
150. C. Palmer, M. Tarazkar, M.J. Gordon, H. Metiu, E.W. McFarland, Methane pyrolysis in low-cost, alkali-halide molten salts at high temperatures, *Sustainable Energy Fuels* **5** (2021) 6107–6123. DOI: 10.1039/d1se01408k
151. H. Papananou, R. Katsumata, Z. Neary, R. Goh, X. Meng, R. Limary, R.A. **Segalman**, Dopamine-mediated polymer coating facilitates area-selective atomic layer deposition, *ACS Appl. Polym. Mater.* **3** (2021) 4924–4931. DOI: 10.1021/acsapm.1c00692

152. T.N. Pardue, M. Goyal, B. Guo, S. Salmani-Rezaie, H. Kim, O. Heinonen, M.D. Johannes, S. Stemmer, Controlling the symmetry of cadmium arsenide films by epitaxial strain, *APL Mater.* **9** (2021) 051111. DOI: 10.1063/5.0047933
153. K. Parto, S.I. Azzam, K. Banerjee, G. Moody, Defect and strain engineering of monolayer WSe<sub>2</sub> enables site-controlled single-photon emission up to 150 K, *Nat. Commun.* **12** (2021) 3585. DOI: 10.1038/s41467-021-23709-5
154. K. Parto, A. Pal, T. Chavan, K. Agashiwala, C-H. Yeh, W. Cao, K. Banerjee, One-dimensional edge contacts to two-dimensional transition-metal dichalcogenides: Uncovering the role of Schottky-Barrier anisotropy in charge transport across MoS<sub>2</sub>/metal interfaces, *Phys. Rev. Appl.* **15** (2021) 064068. DOI: 10.1103/PhysRevApplied.15.064068
155. J.A. Peterson, F. Stricker, J. **Read de Alaniz**, Improving the kinetics and dark equilibrium of donor–acceptor Stenhouse adduct by triene backbone design, *Chem. Commun.* **58** (2022) 2303. DOI: 10.1039/d1cc06235b
156. N. Picciani, J.R. Kerlin, K. Jindrich, N.M. Hensley, D.A. Gold, T.H. Oakley, Light modulated cnidocyte discharge predates the origins of eyes in Cnidaria, *Ecol. Evol.* **11** (2021) 3933–3940. DOI: 10.1002/ece3.7280
157. G. Pokharel, S.M.L. Teicher, B.R. Ortiz, P.M. Sarte, G. Wu, S. Peng, J. He, R. **Seshadri**, S.D. **Wilson**, Electronic properties of the topological kagome metals YV<sub>6</sub>Sn<sub>6</sub> and GdV<sub>6</sub>Sn<sub>6</sub>, *Phys. Rev. B* **104** (2021) 235139. DOI: 10.1103/PhysRevB.104.235139
158. Z. Porter, E. Zoghlin, J.L. Schmehr, S.D. **Wilson**, Crystal growth of Sr<sub>2</sub>Ir<sub>x</sub>Ru<sub>1-x</sub>O<sub>4</sub> for  $\chi \leq 0.4$ , *J. Cryst. Growth* **578** (2022) 126432. DOI: 10.1016/j.jcrysgro.2021.126432
159. T. Prasopdee, C. Sinthuvanich, R. Chollakup, P. Uttayarat, W. Smithipong, The albumin/starch scaffold and its biocompatibility with living cells, *Mater. Today Commun.* **27** (2021) 102164. DOI: 10.1016/j.mtcomm.2021.102164
160. M.B. Preefer, J.H. Grebenkemper, C.E. Wilson, M. Everingham, J.A. Cooley, R. **Seshadri**, Subtle local structural details influence ion transport in glassy Li<sup>+</sup> thiophosphate solid electrolytes, *ACS Appl. Mater. Interfaces* **13** (2021) 57567–57575. DOI: 10.1021/acsami.1c16515
161. E. Pretti, M.S. Shella, A microcanonical approach to temperature-transferable coarse-grained models using the relative entropy, *J. Chem. Phys.* **155** (2021) 094102. DOI: 10.1063/5.0057104
162. N. Ratcliff, L. Hallett, B.R. Ortiz, S.D. **Wilson**, J.W. Harter, Coherent phonon spectroscopy and interlayer modulation of charge density wave order in the kagome metal CsV<sub>3</sub>Sb<sub>5</sub>, *Phys. Rev. Mater.* **5** (2021) L111801. DOI: 10.1103/PhysRevMaterials.5.L111801
163. D. Rawlings, D. Lee, J. Kim, I-B. Magdău, G. Pace, P.M. Richardson, E.M. Thomas, S.P.O. Danielsen, S.H. Tolbert, T.F. Miller, R. **Seshadri**, R.A. **Segalman**, Li<sup>+</sup> and oxidant addition to control ionic and electronic conduction in ionic liquid-functionalized conjugated polymers, *Chem. Mater.* **33** (2021) 6464–6474. DOI: 10.1021/acs.chemmater.1c01811
164. G.N.M. Reddy, P. Selter, Y. Makita, S. Arai, M. Miyagawa, H. Nakano, H. Wang, J.A. Gerbec, F. Shimizu, B.F. **Chmelka**, Nanoscale surface compositions and structures of plasma-modified poly(ethylene terephthalate) thin films, *J. Phys. Chem. C* **125** (2021) 20658–20669. DOI: 10.1021/acs.jpcc.1c06658

165. C.E. Reilly, N. Hatui, T.E. Mates, P. Koirala, A.A. Oni, S. Nakamura, S.P. DenBaars, S. Keller, Properties of AlN/GaN heterostructures grown at low growth temperatures with ammonia and dimethylhydrazine, *Crystals* **11** (2021) 1412. DOI: 10.3390/crust11111412
166. C.E. Reilly, N. Hatui, T.E. Mates, S. Nakamura, S.P. DenBaars, S. Keller, 2DEGs formed in AlN/GaN HEMT structures with AlN grown at low temperature, *Appl. Phys. Lett.* **118** (2021) 222103. DOI: 10.1063/5.0050584
167. L.L. Robinson, J.L. Self, A.D. Fusi, M.W. Bates, J. **Read de Alaniz**, C.J. **Hawker**, C.M. **Bates**, C.S. Sample, Chemical and mechanical tunability of 3D-printed dynamic covalent networks based on boronate esters, *ACS Macro Lett.* **10** (2021) 857–863. DOI: 10.1021/acsmacrolett.1c00257
168. B. Roehrich, E.Z. Liu, R. Silverstein, L. Sepunaru, Detection and characterization of single particles by electrochemical impedance spectroscopy, *J. Phys. Chem. Lett.* **12** (2021) 9748–9753. DOI: 10.1021/acs.jpclett.1c02822
169. R.A. Romero, S. Xu, W-R. Jian, I.J. Beyerlein, C.V. Ramana, Atomistic simulations of the local slip resistances in four refractory multi-principal element alloys, *Int. J. Plast.* **149** (2022) 103157. DOI: 10.1016/j.ijplas.2021.103157
170. A.J.E. Rowberg, S. Mu, M.W. Swift, C.G. Van de Walle, Structural, electronic, and polarization properties of YN and LaN, *Phys. Rev. Mater.* **5** (2021) 094602. DOI: 10.1103/PhysRevMaterials.5.094602
171. A.J.E. Rowberg, M.W. Swift, C.G. Van de Walle, Understanding carbon contamination in the proton-conducting zirconates and cerates, *Phys. Chem. Chem. Phys.* **23** (2021) 14205–14211. DOI: 10.1039/D1CP01902C
172. A.J.E. Rowberg, C.G. Van de Walle, Hydride conductivity in nitride hydrides, *ACS Appl. Energy Mater.* **4** (2021) 6348–6355. DOI: 10.1021/acsaem.1c01208
173. M. Saber, M.B. Peefer, S.K. Kolli, W. Zhang, G. Laurita, B. Dunn, R. **Seshadri**, A. **Van der Ven**, Role of electronic structure in Li ordering and chemical strain in the fast charging Wadsley–Roth phase PN<sub>9</sub>O<sub>25</sub>, *Chem. Mater.* **33** (2021) 7755–7766. DOI: 10.1021/acs.chemmater.1c02059
174. S. Şalap-Ayça, P. Jankowski, K.C. Clarke, A. Nara, Is less more? Experimenting with visual stacking of coincident maps for spatial global sensitivity analysis in urban land-use change modeling, *Environ. Modell. Software* **145** (2021) 105181. DOI: 10.1016/j.envsoft.2021.105181
175. S. Salmani-Rezaie, L. Galletti, T. Schumann, R. Russell, H. Jeong, Y. Li, J. W. Harter, S. Stemmer, Superconductivity in magnetically doped SrTiO<sub>3</sub>, *Appl. Phys. Lett.* **118** (2021) 202602. DOI: 10.1063/5.0052319
176. S. Salmani-Rezaie, H. Jeong, R. Russell, J.W. Harter, S. Stemmer, Role of locally polar regions in the superconductivity of SrTiO<sub>3</sub>, *Phys. Rev. Mater.* **5** (2021) 104801. DOI: 10.1103/PhysRevMaterials.5.104801
177. S. Sang, Y. Li, T. Zhou, X. Chen, T.H. Hsieh, M.P.A. Fisher, Entanglement negativity at measurement-induced criticality, *PRX Quantum* **2** (2021) 030313. DOI: 10.1103/PRXQuantum.2.030313

178. J. Sarver, E. Schultz, A. Apigo, D.S. Gernandt, R. Salas-Lizana, R. Oono, Deep sequencing across multiple host species tests pine-endophyte specificity, *Am. J. Bot.* **109** (2022) 83–98. DOI: 10.1002/ajb2.1792
179. R. Satish, L. Wichmann, M.J. Crafton, R. Giovine, L. Li, J. Ahn, Y. Yue, W. Tong, G. Chen, C. Wang, R.J. Clément, R. Kostecki, Exposure history and its effect towards stabilizing Li exchange across disordered rock salt interfaces, *ChemElectroChem* **8** (2021) 3982–3991. DOI: 10.1002/celc.202100891
180. E.C. Schueller, Y.M. Oey, K.D. Miller, K.E. Wyckoff, R. Zhang, W. Zhang, S.D. Wilson, J.M. Rondinelli, R. Seshadri, AB<sub>2</sub>X<sub>6</sub> compounds and the stabilization of trirutile oxides, *Inorg. Chem.* **60** (2021) 9224–9232. DOI: 10.1021/acs.inorgchem.1c01366
181. W.C. Schultz, L. Bildsten, Y-F. Jiang, Stochastic low-frequency variability in three-dimensional radiation hydrodynamical models of massive star envelopes, *Astrophys. J. Lett.* **924** (2022) L11. DOI: 10.3847/2041-8213/ac441f
182. J.L. Self, V.G. Reynolds, J. Blankenship, E. Mee, J. Guo, K. Albanese, R. Xie, C.J. Hawker, J. Read de Alaniz, M.L. Chabinyc, C.M. Bates, Carbon nanotube composites with bottlebrush elastomers for compliant electrodes, *ACS Polym. Au* **2** (2022) 27–34. DOI: 10.1021/acspolymersau.1c00034
183. J. Selvidge, E.T. Hughes, J.C. Norman, C. Shang, M.J. Kennedy, M. Dumont, A.M. Netherton, Z. Zhang, R.W. Herrick, J.E. Bowers, K. Mukherjee, Reduced dislocation growth leads to long lifetime InAs quantum dot lasers on silicon at high temperatures, *Appl. Phys. Lett.* **118** (2021) 192101. DOI: 10.1063/5.0052316
184. A.D. Sezer, U. Madhow, M.J.W. Rodwell, ‘Spatial oversampling for quantized LoS MIMO’, *2021 55th Asilomar Conference on Signals, Systems, and Computers*, October 31–November 3, 2021, Pacific Grove, CA. Pages 405–409 (2021). DOI: 10.1109/IEEECONF53345.2021.9723314
185. Y. Shen, A. Pressman, E. Janzen, I.A. Chen, Kinetic sequencing (*k*-Seq) as a massively parallel assay for ribozyme kinetics: Utility and critical parameters, *Nucleic Acids Res.* **49** (2021) e67. DOI: 10.1093/nar/gkab199
186. N. Sherck, K. Shen, M. Nguyen, B. Yoo, S. Köhler, J.C. Speros, K.T. Delaney, M.S. Shell, G.H. Fredrickson, Molecularly informed field theories from bottom-up coarse-graining, *ACS Macro Lett.* **10** (2021) 576–583. DOI: 10.1021/acsmacrolett.1c00013
187. I.A. Shojaei, S. Pournia, C. Le, B.R. Ortiz, G. Jnawali, F-C. Zhang, S.D. Wilson, H.E. Jackson, L.M. Smith, A Raman probe of phonons and electron–phonon interactions in the Weyl semimetal NbIrTe<sub>4</sub>, *Sci. Rep.* **11** (2021) 8155. DOI: 10.1038/s41598-021-87302-y
188. O.F. Shoron, D.A. Kealhofer, M. Goyal, T. Schumann, A.A. Burkov, S. Stemmer, Detecting topological phase transitions in cadmium arsenide films via the transverse magnetoresistance, *Appl. Phys. Lett.* **119** (2021) 171907. DOI: 10.1063/5.0066252
189. N. Shumiya, Md.S. Hossain, J.-X. Yin, Y.-X. Jiang, B.R. Ortiz, H. Liu, Y. Shi, Q. Yin, H. Lei, S.S. Zhang, G. Chang, Q. Zhang, T.A. Cochran, D. Multer, M. Litskevich, Z.-J. Cheng, X.P. Yang, Z. Guguchia, S.D. Wilson, M.Z. Hasan, Intrinsic nature of chiral charge order in the kagome superconductor RbV<sub>3</sub>Sb<sub>5</sub>, *Phys. Rev. B* **104** (2021) 35131. DOI: 10.1103/PhysRevB.104.035131

190. R. Silverstein, F.W. Zok, C.G. Levi, Vapor-mediated melt infiltration for synthesizing SiC composite matrices, *J. Am. Ceram. Soc.* **104** (2021) 3833–3844. DOI: 10.1111/jace.17793
191. R. Singha, T.H. Salters, S.M.L. Teicher, S. Lei, J.F. Khouri, N.P. Ong, L.M. Schoop, Evolving devil's staircase magnetization from tunable charge density waves in nonsymmorphic Dirac semimetals, *Adv. Mater.* **33** (2021) 2103476. DOI: 10.1002/adma.202103476
192. R. Singha, F. Yuan, G. Cheng, T.H. Salters, Y.M. Oey, G.V. Villalpando, M. Jovanovic, N. Yao, L.M. Schoop, TaCo<sub>2</sub>Te<sub>2</sub>: An air-stable, high mobility Van der Waals material with probable magnetic order, *Adv. Funct. Mater.* **32** (2022) 2108920. DOI: 10.1002/adfm.202108920
193. I. Spanopoulos, I. Hadar, W. Ke, P. Guo, E.M. Mozur, E. Morgan, S. Wang, D. Zheng, S. Padgaonkar, G.N.M. Reddy, E.A. Weiss, M.C. Hersam, R. **Seshadri**, R.D. Schaller, M.G. Kanatzidis, Tunable broad light emission from 3D “hollow” bromide perovskites through defect engineering, *J. Am. Chem. Soc.* **143** (2021) 7069–7080. DOI: 10.1021/jacs.1c01727
194. M.M. Sroda, F. Stricker, J.A. Peterson, A. Bernal, J. **Read de Alaniz**, Donor–acceptor Stenhouse adducts: Exploring the effects of ionic character, *Chem. Eur. J.* **27** (2021) 4183–4190. DOI: 10.1002/chem.202005110  
(Published 24 February 2021. This paper was missed when compiling last year's report.)
195. S.L. Staun, G. Wu, W.W. Lukens, T.W. Hayton, Synthesis of a heterobimetallic actinide nitride and an analysis of its bonding, *Chem. Sci.* **12** (2021) 15519–15527. DOI: 10.1039/D1SC05072A
196. C. Swindle, P. Shankin-Clarke, M. Meyerhof, J. Carlson, J. Melac, Effects of wildfires and ash leaching on stream chemistry in the Santa Ynez mountains of Southern California, *Water* **13** (2021) 2402. DOI: 10.3390/w13172402
197. H. Tan, A. Banerjee, N. Shi, X. Tang, A. Abdel-Fattah, T.M. Squires, A two-step strategy for delivering particles to targets hidden within microfabricated porous media, *Sci. Adv.* **7** (2021) eabh0638. DOI: 10.1126/sciadv.abh0638
198. J.C. Thomas, A.R. Natarajan, A. **Van der Ven**, Comparing crystal structures with symmetry and geometry, *npj Comput. Mater.* **7** (2021) 164. DOI: 10.1038/s41524-021-00627-0
199. M.D. Tikekar, K.T. Delaney, M.C. Villet, D.R. Tree, G.H. **Fredrickson**, A phase field model for dynamic simulations of reactive blending of polymers, *Soft Matter* **18** (2022) 877–893. DOI: 10.1039/D1SM01686E
200. A.J. Touchton, G. Wu, T.W. Hayton, [Ni<sub>23</sub>Se<sub>12</sub>(PEt<sub>3</sub>)<sub>13</sub>] Revisited: Isolation and characterization of [Ni<sub>23</sub>Se<sub>12</sub>Cl<sub>3</sub>(PEt<sub>3</sub>)<sub>10</sub>], *Inorg. Chem.* **60** (2021) 17586–17592. DOI: 10.1021/acs.inorgchem.1c02184
201. A.J. Touchton, G. Wu, T.W. Hayton, [Ni<sub>8</sub>(CN<sup>t</sup>Bu)<sub>12</sub>][Cl]: A nickel isocyanide nanocluster with a folded nanosheet structure, *J. Chem. Phys.* **154** (2021) 211102. DOI: 10.1063/5.0054231
202. A.J. Touchton, G. Wu, T.W. Hayton, Synthesis of bis(trityl)iron(II) and formation of the iron(0)-stabilized o,o-isomer of Gomberg's dimer, *Organometallics* **40** (2021) 4045–4049. DOI: 10.1021/acs.organomet.1c00616
203. A.J. Touchton, G. Wu, T.W. Hayton, Understanding the early stages of nickel sulfide

- nanocluster growth: Isolation of Ni<sub>3</sub>, Ni<sub>4</sub>, Ni<sub>5</sub>, and Ni<sub>8</sub> intermediates, *Small* **17** (2021) 2003133. DOI: 10.1002/smll.202003133
204. H-Y. Tseng, Y. Fang, W.J. Mitchell, A.A. Taylor, M.J.W. Rodwell, Atomic layer deposition of TiN/Ru gate in InP MOSFETs, *Appl. Phys. Lett.* **119** (2021) 123502. DOI: 10.1063/5.0058825
205. D.L. Vigil, K.T. Delaney, G.H. Fredrickson, Quantitative comparison of field-update algorithms for polymer SCFT and FTS, *Macromolecules* **54** (2021) 9804–9814. DOI: 10.1021/acs.macromol.1c01804
206. R.C. Vincent, J-X. Shen, M.B. Peefer, J. Lin, F. Seeler, K. Schierle-Arndt, K.A. Persson, R. Seshadri, Prospects for employing lithium copper phosphates as high-voltage Li-Ion cathodes, *J. Phys. Chem. C* **125** (2021) 13123–13130. DOI: 10.1021/acs.jpcc.1c01406
207. P. Vishnoi, J.L. Zuo, J.A. Cooley, L. Kautzsch, A. Gómez-Torres, J. Murillo, S. Fortier, S.D. Wilson, R. Seshadri, A.K. Cheetham, Chemical control of spin-orbit coupling and charge transfer in vacancy-ordered ruthenium(IV) halide perovskites, *Angew. Chem. Int. Ed.* **60** (2021) 5184–5188. DOI: 10.1002/anie.202013383
208. H. Wang, N. Adamski, S. Mu, C.G. Van de Walle, Piezoelectric effect and polarization switching in Al<sub>1-x</sub>Sc<sub>x</sub>N, *J. Appl. Phys.* **130** (2021) 104101. DOI: 10.1063/5.0056485
209. J. Wang, K.F. Jorgensen, E. Farzana, K.S. Qwah, M. Monavarian, Z.J. Biegler, T. Mates, J.S. Speck, Impact of growth parameters on the background doping of GaN films grown by ammonia and plasma-assisted molecular beam epitaxy for high-voltage vertical power switches, *APL Mater.* **9** (2021) 081118. DOI: 10.1063/5.0060154
210. J. Wang, B.K. SaifAddin, C.J. Zollner, B. Bonef, A.S. Almogbel, Y. Yao, M. Iza, Y. Zhang, M.N. Fireman, E.C. Young, S.P. DenBaars, S. Nakamura, J.S. Speck, High conductivity n-Al<sub>0.6</sub>Ga<sub>0.4</sub>N by ammonia-assisted molecular beam epitaxy for buried tunnel junctions in UV emitters, *Opt. Express* **29** (2021) 40781–40794. DOI: 10.1364/OE.436153
211. M. Wang, S. Mu, C.G. Van de Walle, Adsorption and diffusion of aluminum on β-Ga<sub>2</sub>O<sub>3</sub>(010) surfaces, *ACS Appl. Mater. Interfaces* **13** (2021) 10650–10655. DOI: 10.1021/acsami.0c22737
212. M. Wang, S. Mu, C.G. Van de Walle, Incorporation of Si and Sn donors in β-Ga<sub>2</sub>O<sub>3</sub> through surface reconstructions, *J. Appl. Phys.* **130** (2021) 185703. DOI: 10.1063/5.0068875
213. X. Wang, S. Xu, W-R. Jian, X.-G. Li, Y. Su, I.J. Beyerlein, Generalized stacking fault energies and Peierls stresses in refractory body-centered cubic metals from machine learning-based interatomic potentials, *Comput. Mater. Sci.* **192** (2021) 110364. DOI: 10.1016/j.commatsci.2021.110364
214. Y. Wang, B. Feng, Y. Ding, 'DSXplore: Optimizing convolutional neural networks via sliding-channel convolutions', *2021 IEEE Intl. Parallel and Distributed Processing Symposium (IPDPS)* (2021) 619–628. May 17–21, 2021, Portland, OR. DOI: 10.1109/IPDPS49936.2021.00070
215. Y. Wang, B. Feng, X. Peng, Y. Ding, 'An efficient quantitative approach for optimizing convolutional neural networks', *Proceedings of the 30th ACM Intl. Conf. on Information and Knowledge Management (CIKM '21)*, November 1–5, 2021, Virtual Event, Australia. ACM: New York, NY, USA, 10 pages. DOI: 10.1145/3459637.3482230

216. C. Wangsanuwat, A. Chialastri, J.F. Aldeguer, N.C. Rivron, S.S. Dey, A probabilistic framework for cellular lineage reconstruction using integrated single-cell 5-hydroxymethylcytosine and genomic DNA sequencing, *Cell Rep. Methods* **1** (2021) 100060. DOI: 10.1016/j.crmeth.2021.100060.
217. S.J. Warnock, R. Sujanani, E.S. Zofchak, S. Zhao, T.J. Dilenschneider, K.G. Hanson, S. Mukherjee, V. Ganesan, B.D. Freeman, M.M. Abu-Omar, C.M. **Bates**, Engineering Li/Na selectivity in 12-Crown-4-functionalized polymer membranes, *Proc. Natl. Acad. Sci.* **118** (2021) e2022197118. DOI: 10.1073/pnas.2022197118
218. G. Weng, V. **Vlček**, Efficient treatment of molecular excitations in the liquid phase environment via stochastic many-body theory, *J. Chem. Phys.* **155** (2021) 054104. DOI: 10.1063/5.0058410
219. T.L.S. Wong, L. Bildsten, Mass transfer and stellar evolution of the white dwarfs in AM CVn binaries, *Astrophys. J.* **923** (2021) 125. DOI: 10.3847/1538-4357/ac2b2a
220. T.L.S. Wong, J. Schwab, Y. Götberg, Pre-explosion properties of helium star donors to thermonuclear supernovae, *Astrophys. J.* **922** (2021) 241. DOI: 10.3847/1538-4357/ac27ae
221. W. Wu, N.G. Combs, S. Stemmer, Molecular beam epitaxy of phase-pure antiperovskite Sr<sub>3</sub>SnO thin films, *Appl. Phys. Lett.* **119** (2021) 161903. DOI: 10.1063/5.0068187
222. R. Xie, S. Mukherjee, A.E. Levi, J.L. Self, H. Wang, M.L. **Chabiny**, C.M. **Bates**, Yielding behavior of bottlebrush and linear block copolymers, *Macromolecules* **54** (2021) 5636–5647. DOI: 10.1021/acs.macromol.1c00557
223. S. Xu, J.Y. Cheng, Z. Li, N.A. Mara, I.J. Beyerlein, Phase-field modeling of the interactions between an edge dislocation and an array of obstacles, *Comput. Methods Appl. Mech. Eng.* **389** (2022) 114426. DOI: 10.1016/j.cma.2021.114426
224. S. Xu, W-R. Jian, Y. Su, I.J. Beyerlein, Line-length-dependent dislocation glide in refractory multi-principal element alloys, *Appl. Phys. Lett.* **120** (2022) 061901. DOI: 10.1063/5.0080849
225. Y. Xuan, K.T. Delaney, H.D. Ceniceros, G.H. **Fredrickson**, Deep learning and self-consistent field theory: A path towards accelerating polymer phase discovery, *J. Comput. Phys.* **443** (2021) 110519. DOI: 10.1016/j.jcp.2021.110519
226. (a) R. Yang, S. Yue, Y. Quan, B. **Liao**, Crystal symmetry based selection rules for anharmonic phonon-phonon scattering from a group theory formalism, *Phys. Rev. B* **103** (2021) 184302. DOI: 10.1103/PhysRevB.103.184302
226. (b) R. Yang, S. Yue, Y. Quan, B. **Liao**, **Erratum:** Crystal symmetry based selection rules for anharmonic phonon-phonon scattering from a group theory formalism, *Phys. Rev. B* **104** (2021) 099902. DOI: 10.1103/PhysRevB.104.099902
227. B. Yu, R. Li, R.A. **Segalman**, Tuning the double gyroid phase window in block copolymers via polymer chain conformation near the interface, *Macromolecules* **54** (2021) 5388–5396. DOI: 10.1021/acs.macromol.1c00048
228. Y. Yue, Y. Ha, R. Giovine, R. **Clément**, W. Yang, W. Tong, High-voltage reactivity and long-term stability of cation-disordered rocksalt cathodes, *Chem. Mater.* **34** (2022) 1524–1532. DOI: 10.1021/acs.chemmater.1c03115
229. G. Zakem, I. Ro, J. Finzel, P. Christopher, Support functionalization as an approach for modifying activation entropies of catalytic reactions on atomically dispersed metal sites,

*J. Catal.* **404** (2021) 883–896. DOI: 10.1016/j.jcat.2021.07.030

230. J. Zeng, M. Tarazkar, C. Palmer, M.J. Gordon, H. Metiu, E.W. McFarland, Initial steps in CH<sub>4</sub> pyrolysis on Cu and Ni, *J. Phys. Chem. C* **125** (2021) 18665–18672. DOI: 10.1021/acs.jpcc.1c03606
231. M. Zeng, Y.-H. Lee, G. Strong, A.M. LaPointe, A.L. Kocen, Z. Qu, G.W. Coates, S.L. Scott, M.M. Abu-Omar, Chemical upcycling of polyethylene to value-added  $\alpha,\omega$ -divinyl-functionalized oligomers, *ACS Sustainable Chem. Eng.* **9** (2021) 13926–13936. DOI: 10.1021/acssuschemeng.1c05272
232. J. Zhang, A. Jurzyk, M.E. Helgeson, L.G. Leal, Modeling orthogonal superposition rheometry to probe nonequilibrium dynamics of entangled polymers, *J. Rheol.* **65** (2021) 983. DOI: 10.1122/8.0000272
233. L. Zhang, O. Blaes, Y.-F. Jiang, Radiative MHD simulations of photon bubbles in radiation-supported magnetized atmospheres of neutron stars with isotropic Thomson scattering, *Mon. Not. R. Astron. Soc.* **508** (2021) 617–636. DOI: 10.1093/mnras/stab2510
234. P. Zhang, S.-K. Jian, C. Liu, X. Chen, Emergent replica conformal symmetry in non-Hermitian SYK<sub>2</sub> chains, *Quantum* **5** (2021) 579. DOI: 10.22331/q-2021-11-16-579
235. Y. Zhang, E.C. Self, B.P. Thapaliya, R. Giovine, H.M. Meyer, L. Li, Y. Yue, D. Chen, W. Tong, G. Chen, C. Wang, R. Clément, S. Dai, J. Nanda, Formation of LiF surface layer during direct fluorination of high-capacity co-free disordered rocksalt cathodes, *ACS Appl. Mater. Interfaces* **13** (2021) 38221–38228. DOI: 10.1021/acsami.1c07882
236. H. Zhao, H. Li, B.R. Ortiz, S.M.L. Teicher, T. Park, M. Ye, Z. Wang, L. Balents, S.D. Wilson, I. Zeljkovic, Cascade of correlated electron states in the kagome superconductor CsV<sub>3</sub>Sb<sub>5</sub>, *Nature* **599** (2021) 216–221. DOI: 10.1038/s41586-021-03946-w
237. Y. Zhao, E.E. Taylor, X. Hu, B. Evanko, X. Zeng, H. Wang, R. Ohnishi, T. Tsukazaki, J.-F. Li, N.P. Stadie, S.J. Yoo, G.D. Stucky, S.W. Boettcher, What structural features make porous carbons work for redox-enhanced electrochemical capacitors? A fundamental investigation, *ACS Energy Lett.* **6** (2021) 854–861. DOI: 10.1021/acsenergylett.0c02424
238. Y. Zhen, K.K. Ewert, W.S. Fisher, V.M. Steffes, Y. Li, C.R. Safinya, Paclitaxel loading in cationic liposome vectors is enhanced by replacement of oleoyl with linoleoyl tails with distinct lipid shapes, *Sci. Rep.* **11** (2021) Article number: 7311. DOI: 10.1038/s41598-021-86484-9
239. T. Zhou, X. Chen, Nonunitary entanglement dynamics in continuous-variable systems, *Phys. Rev. B* **104** (2021) L180301. DOI: 10.1103/PhysRevB.104.L180301
240. E.S. Zofchak, Z. Zhang, B.K. Wheatle, R. Sujanani, S.J. Warnock, T.J. Dilenschneider, K.G. Hanson, S. Zhao, S. Mukherjee, M.M. Abu-Omar, C.M. Bates, B.D. Freeman, V. Ganesan, Origins of lithium/sodium reverse permeability selectivity in 12-crown-4-functionalized polymer membranes, *ACS Macro Lett.* **10** (2021) 1167–1173. DOI: 10.1021/acsmacrolett.1c00243
241. E. Zoghlin, J. Schmehr, C. Holgate, R. Dally, Y. Liu, G. Laurita, S.D. Wilson, Evaluating the effects of structural disorder on the magnetic properties of Nd<sub>2</sub>Zr<sub>2</sub>O<sub>7</sub>, *Phys. Rev. Mater.* **5** (2021) 084403. DOI: 10.1103/PhysRevMaterials.5.084403