

LIST OF MRSEC-SUPPORTED PUBLICATIONS

2019-2020 [213]

Mar. 1, 2019 – Feb. 29, 2020

IRG-1 [11]

a. Primary MRSEC Support that Acknowledge the MRSEC Award DMR-1720256 [5]

1. E. Decolvenaere, E. Levin, R. **Seshadri**, A. **Van der Ven**, Modeling magnetic evolution and exchange hardening in disordered magnets: The example of $Mn_{1-x}Fe_xRu_2Sn$ Heusler alloys, *Phys. Rev. Mater.* **3** (2019) 104411. DOI: 10.1103/PhysRevMaterials.3.104411
2. L. Kautzsch, J.D. Bocarsly, C. Felser, S.D. **Wilson**, R. **Seshadri**, Controlling Dzyaloshinskii-Moriya interactions in the skyrmion host candidates $FePd_{1-x}Pt_xMo_3N$, *Phys. Rev. Mater.* **4** (2020) 024412. DOI: 10.1103/PhysRevMaterials.4.024412
3. D.A. Kitchaev, E.C. Schueller, A. **Van der Ven**, Mapping skyrmion stability in uniaxial lacunar spinel magnets from first principles, *Phys. Rev. B* **101** (2020) 054409. DOI: 10.1103/PhysRevB.101.054409
4. E.E. Levin, J.H. Grebenkemper, T.M. **Pollock**, R. **Seshadri**, Protocols for high temperature assisted-microwave preparation of inorganic compounds, *Chem. Mater.* **31** (2019) 7151–7159. DOI: 10.1021/acs.chemmater.9b02594
5. J.C. Stinville, E.R. Yao, P.G. Callahan, J. Shin, F. Wang, M.P. Echlin, T.M. **Pollock**, D.S. **Gianola**, Dislocation dynamics in a nickel-based superalloy via in-situ transmission scanning electron microscopy, *Acta Mater.* **168** (2019) 152–166. DOI: 10.1016/j.actamat.2018.12.061

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

6. J.D. Bocarsly, E.E. Levin, S.A. Humphrey, T. Faske, W. Donner, S.D. **Wilson**, R. **Seshadri**, Magnetostructural coupling drives magnetocaloric behavior: The case of MnB versus FeB, *Chem. Mater.* **31** (2019) 4873–4881. DOI: 10.1021/acs.chemmater.9b01476
7. D. **Gianola**, T. Britton, S. Zaefferer, New techniques for imaging and identifying defects in electron microscopy, *MRS Bull.* **44** (2019) 450–458. DOI: 10.1557/mrs.2019.125
8. M.I. Latypov, M-A. Charpagne, M. Souther, B.R. Goodlet, M.P. Echlin, I.J. Beyerlein,

- T.M. **Pollock**, Computational homogenization for multiscale forward modeling of resonant ultrasound spectroscopy of heterogeneous materials, *Mater. Charact.* **158** (2019) 109945. DOI: 10.1016/j.matchar.2019.109945
9. K. Pilar, Z. Deng, M.B. Preefer, J.A. Cooley, R. **Clément**, R. **Seshadri**, A.K. Cheetham, Ab initio computation for solid-state ^{31}P NMR of inorganic phosphates: Revisiting X-ray structures, *Phys. Chem. Chem. Phys.* **21** (2019) 10070–10074. DOI: 10.1039/c9cp01420a
 10. E.C. Schueller, J.L. Zuo, J.D. Bocarsly, D.A. Kitchaev, S.D. **Wilson**, R. **Seshadri**, Modeling the structural distortion and magnetic ground state of the polar lacunar spinel GaV_4Se_8 , *Phys. Rev. B* **100** (2019) 045131. DOI: 10.1103/PhysRevB.100.045131
 11. J. Shin, L.Y. Chen, U.T. Sanli, G. Richter, S. Labat, M-I. Richard, T. Cornelius, O. Thomas, D.S. **Gianola**, Controlling dislocation nucleation-mediated plasticity in nanostructures via surface modification, *Acta Mater.* **166** (2019) 572e586. DOI: 10.1016/j.actamat.2018.12.048

IRG-2 [9]

a. Primary MRSEC Support that Acknowledge the MRSEC Award DMR-1720256 [5]

12. D.J. Grzetic, K.T. Delaney, G.H. **Fredrickson**, Field-theoretic study of salt-induced order and disorder in a polarizable diblock copolymer, *ACS Macro Lett.* **8** (2019) 962–967. DOI: 10.1021/acsmacrolett.9b00316
13. C.S. Sample, S-H. Lee, M.W. Bates, J.M. Ren, J. Lawrence, V. Lensch, J.A. Gerbec, C.M. **Bates**, S. Li, C.J. **Hawker**, Metal-free synthesis of poly(silyl ether)s under ambient conditions, *Macromolecules* **52** (2019) 1993–1999. DOI: 10.1021/acs.macromol.8b02741
14. C.S. Sample, S-H. Lee, S. Li, M.W. Bates, V. Lensch, B.A. Versaw, C.M. **Bates**, C.J. **Hawker**, Metal-free room-temperature vulcanization of silicones via borane hydrosilylation, *Macromolecules* **52** (2019) 7244–7250. DOI: 10.1021/acs.macromol.9b01585
15. N.S. Schausser, R. **Seshadri**, R.A. **Segalman**, Multivalent ion conduction in solid polymer systems, *Mol. Syst. Des. Eng.* **4** (2019) 263. DOI: 10.1039/c8me00096d
16. M.S. Zayas, N.D. Dolinski, J.L. Self, A. Abdilla, C.J. **Hawker**, C.M. **Bates**, J. **Read de Alaniz**, Tuning merocyanine photoacid structure to enhance solubility and temporal control: Application in ring opening polymerization, *Chem Photo Chem* **3** (2019) 467–472. Special Issue: Photoresponsive Molecular Switches and Machines DOI: 10.1002/cptc.201800255

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17. A.V. Bayles, C.S. Valentine, T. Üherrück, S.P.O. Danielsen, S. **Han**, M.E. **Helgeson**, T.M. **Squires**, Anomalous solute diffusivity in ionic liquids: Label-free visualization and physical origins, *Phys. Rev. X* **9** (2019) 011048. DOI: 10.1103/PhysRevX.9.011048
18. D.J. Grzetic, K.T. Delaney, G.H. **Fredrickson**, Contrasting dielectric properties of electrolyte solutions with polar and polarizable solvents, *Phys. Rev. Lett.* **122** (2019) 128007. DOI: 10.1103/PhysRevLett.122.128007
19. H. Nie, J.L. Self, A.S. Kuenstler, R.C. Hayward, J. **Read de Alaniz**, Multiaddressable photochromic architectures: From molecules to materials, *Adv. Opt. Mater.* **7** (2019) 1900224. DOI: 10.1002/adom.201900224
20. A.H. St. Amant, E.H. Discekici, S.J. Bailey, M.S. Zayas, J-A. Song, S.L. Shankel, S.N. Nguyen, M.W. Bates, A. Anastasaki, C.J. **Hawker**, J. **Read de Alaniz**, Norbornadienes: Robust and scalable building blocks for cascade “click” coupling of high molecular weight polymers, *J. Am. Chem. Soc.* **141** (2019) 13619–13624. DOI: 10.1021/jacs.9b06328

IRG-3 [14]

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

21. S.M. Barbon, N.P. Truong, A.G. Elliott, M.A. Cooper, T.P. Davis, M.R. Whittaker, C.J. **Hawker**, A. Anastasaki, Elucidating the effect of sequence and degree of polymerization on antimicrobial properties for block copolymers, *Polym. Chem.* **11** (2020) 84–90. DOI: 10.1039/C9PY01435G
22. N. Cohen, J.H. **Waite**, R.M. **McMeeking**, M.T. **Valentine**, Force distribution and multiscale mechanics in the mussel byssus, *Phil. Trans. R. Soc. B* **374** (2019) 20190202. DOI: 10.1098/rstb.2019.0202
23. S.P.O. Danielsen, J. McCarty, J-E. **Shea**, K.T. Delaney, G.H. **Fredrickson**, Molecular design of self-coacervation phenomena in block polyampholytes, *PNAS* **116** (2019) 8224–8232. DOI: 10.1073/pnas.1900435116
24. S.P.O. Danielsen, J. McCarty, J-E. **Shea**, K.T. Delaney, G.H. **Fredrickson**, Small ion effects on self-coacervation phenomena in block polyampholytes, *J. Chem. Phys.* **151** (2019) 034904. DOI: 10.1063/1.5109045

25. Z. Geng, J. Lee, C.J. **Hawker**, Placing functionality where you want: The allure of sequence control, *Chem* **5** (2019) 2510–2512. DOI: 10.1016/j.chempr.2019.09.007
26. Y. Lin, J. McCarty, J.N. Rauch, K.T. Delaney, K.S. Kosik, G.H. **Frederickson**, J-E. **Shea**, S. **Han**, Narrow equilibrium window for complex coacervation of tau and RNA under cellular conditions, *eLife* **8** (2019) e42571. DOI: 10.7554/eLife.42571
27. E. Valois, C. Hoffman, D.G. Demartini, J.H. **Waite**, The thiol-rich interlayer in the shell/core architecture of mussel byssal threads, *Langmuir* **35** (2019) 15985–15991. DOI: 10.1021/acs.langmuir.9b01844

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30. P.R. Judzewitsch, N. Corrigan, F. Trujillo, J. Xu, G. Moad, C.J. **Hawker**, E.H.H. Wong, C. Boyer, High-throughput process for the discovery of antimicrobial polymers and their upscaled production via flow polymerization, *Macromolecules* **53** (2020) 631–639. DOI: 10.1021/acs.macromol.9b02207
31. Z.A. Levine, K. Teranishi, A.K. Okada, R. Langen, J-E. **Shea**, The mitochondrial peptide humanin targets but does not denature amyloid oligomers in Type II diabetes, *J. Am. Chem. Soc.* **141** (2019) 14168–14179. DOI: 10.1021/jacs.9b04995
32. J. McCarty, K.T. Delaney, S.P.O. Danielsen, G.H. **Fredrickson**, J-E. **Shea**, Complete phase diagram for liquid–liquid phase separation of intrinsically disordered proteins, *J. Phys. Chem. Lett.* **10** (2019) 1644–1652. DOI: 10.1021/acs.jpcllett.9b00099
33. D.R. Tree, L.F. Dos Santos, C.B. Wilson, T.R. Scott, J.U. Garcia, G.H. **Fredrickson**, Mass-transfer driven spinodal decomposition in a ternary polymer solution, *Soft Matter* **15** (2019) 4614. DOI: 10.1039/c9sm00355j
34. B.J. Walder, N.A. Prisco, F.M. Paruzzo, J.R. Yarava, B.F. **Chmelka**, L. Emsley, Measurement of proton spin diffusivity in hydrated cementitious solids, *J. Phys. Chem. Lett.* **10** (2019) 5064–5069. DOI: 10.1021/acs.jpcllett.9b01861

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a. Primary MRSEC Support that Acknowledge the MRSEC Award DMR-1720256 [4]

35. B. Bonaf, R.D. Shah, K. **Mukherjee**, Fast diffusion and segregation along threading dislocations in semiconductor heterostructures, *Nano Lett.* **19** (2019) 1428–1436. DOI: 10.1021/acs.nanolett.8b03734
36. L. Dong, H. Zhao, I. Zeljkovic, S.D. **Wilson**, J.W. **Harter**, Bulk superconductivity in $\text{FeTe}_{1-x}\text{Se}_x$ via physicochemical pumping of excess iron, *Phys. Rev. Mater.* **3** (2019) 114801. DOI: 10.1103/PhysRevMaterials.3.114801
37. M.E. Turiansky, A. Alkauskas, L.C. Bassett, C.G. **Van de Walle**, Dangling bonds in hexagonal boron nitride as single-photon emitters, *Phys. Rev. Lett.* **123** (2019) 127401. DOI: 10.1103/PhysRevLett.123.127401
38. M.E. Turiansky, J-X. Shen, D. Wickramaratne, C.G. **Van de Walle**, First-principles study of bandgap bowing in B_{0.9}GaN alloys, *J. Appl. Phys.* **126** (2019) 095706. DOI: 10.1063/1.5111414

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42. M. Abdelghany, U. Madhow, M. Rodwell, An efficient digital backend for wideband single-carrier mmWave massive MIMO, *Proceedings from the 2019 IEEE Global Communications Conference (GLOBECOM)*, Dec. 9-13, 2019, Waikoloa, HI, USA (2019) 1-6. DOI: 10.1109/GLOBECOM38437.2019.9013233

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44. N.M. Abdul-Jabbar, A.N. Fernandez, R.W. Jackson, D. Park, W.D. Summers, C.G. Levi, Interactions between zirconia–yttria–tantala thermal barrier oxides and silicate melts, *Acta Mater.* **185** (2020) 171–180. DOI: 10.1016/j.actamat.2019.11.060
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56. N.F. Bouxsein, C. Leal, C.S. McAllister, Y. Li, K.K. Ewert, C.E. Samuel, C.R. Safinya, 3D columnar phase of stacked short DNA organized by coherent membrane undulations, *Langmuir* **35** (2019) 11891–11901. DOI: 10.1021/acs.langmuir.9b01726
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58. S.T.Š. Brunelli, B. Markman, A. Goswami, H-Y. Tseng, S. Choi, C. Palmstrøm, M. Rodwell, J. Klamkin, Selective and confined epitaxial growth development for novel nano-scale electronic and photonic device structures, *J. Appl. Phys.* **126** (2019) 015703. DOI: 10.1063/1.5097174
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61. C-C. Chang, I. Williams, A. Nowbahar, V. Mansard, J. Mecca, K.A. Whitaker, A.K. Schmitt, C.J. Tucker, T.H. Kalantar, T-C. Kuo, T.M. **Squires**, Effect of ethylcellulose on the rheology and mechanical heterogeneity of asphaltene films at the oil–water interface, *Langmuir* **35** (2019) 9374–9381. DOI: 10.1021/acs.langmuir.9b00834

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