

LIST OF MRSEC-SUPPORTED PUBLICATIONS

2017-2018 [33]

Sept. 1, 2017 – Feb. 28, 2018

IRG-1 [2]

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

1. E. Decolvenaere, M. Gordon, R. **Seshadri**, A. **Van der Ven**, "First-principles investigation of competing magnetic interactions in (Mn,Fe) Ru₂Sn Heusler solid solutions," *Phys. Rev. B* **96** (2017) 165109.
DOI: 10.1103/PhysRevB.96.165109
2. E.E. Levin, J.D. Bocarsly, K.E. Wyckoff, T.M. **Pollock**, R. **Seshadri**, "Tuning the magnetocaloric response in half-Heusler/Heusler MnNi_{1-x}Sb solid solutions," *Phys. Rev. Mater.* **1** (2017) 075003.
DOI: 10.1103/PhysRevMaterials.1.075003

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

None

IRG-2 [3]

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

3. J. Bartels, G.E. Sanoja, C.M. Evans, R.A. **Segalman**, M.E. **Helgeson**, "Decoupling mechanical and conductive dynamics of polymeric ionic liquids via a trivalent anion additive," *Macromolecules* **50** (2017) 8979-8987.
DOI: 10.1021/acs.macromol.7b01351
4. I.-H. Lee, E.H. Discekici, S.L. Shankel, A. Anastasaki, J. **Read de Alaniz**, C.J. **Hawker**, D.J. Lunn, "Desulfurization-bromination: Direct chain-end modification of RAFT polymers," *Polym. Chem.* **8** (2017) 7188-7194.
DOI: 10.1039/C7PY01702B
5. J.M. Ren, J. Lawrence, A.S. Knight, A. Abdilla, R. Bou Zerdan, A.E. Levi, B. Oschmann, W.R. Gutekunst, S.-H. Lee, Y. Li, A.J. McGrath, C.M. **Bates**, G.G. Qiao, C.J. **Hawker**, "Controlled formation and binding selectivity of discrete oligo(methyl methacrylate) stereocomplexes," *J. Am. Chem. Soc.* **140** (2018) 1945-1951.

DOI: 10.1021/jacs.7b13095

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

None

IRG-3 [2]

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

6. I. Kaminker, W. Wei, A.M. Schrader, Y. Talmon, M.T. **Valentine**, J.N. Israelachvili, J.H. **Waite**, S. **Han**, "Simple peptide coacervates adapted for rapid pressure-sensitive wet adhesion," *Soft Matter* **13** (2017) 9122-9131.
DOI: 10.1039/C7SM01915G
7. A.S. Knight, J. Larsson, J.M. Ren, R. Bou Zerdan, S. Seguin, R. Vrahas, J. Liu, G. Ren, C.J. **Hawker**, "Control of amphiphile self-assembly via bioinspired metal ion coordination," *J. Am. Chem. Soc.* **140** (2018) 1409-1414.
DOI: 10.1021/jacs.7b11005

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

None

SEED

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

None

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

None

SHARED FACILITIES [26]

8. N.L. Adamski, Z. Zhu, D. Wickramaratne, C.G. **Van de Walle**, "Hybrid functional study of native point defects and impurities in ZnGeN₂," *J. Appl. Phys.* **122** (2017) 195701.
DOI: 10.1063/1.4999790

9. G.C.B. Alexander, D.H. Fabini, R. **Seshadri**, M.G. Kanatzidis, "AuPb₂I₇: A narrow bandgap Au³⁺ iodide semiconductor," *Inorg. Chem.* **57** (2018) 804-810.
DOI: 10.1021/acs.inorgchem.7b02723
10. R. Barnes, S. Sun, Y. Fichou, F.W. Dahlquist, M. Heyden, S. **Han**, "Spatially heterogeneous surface water diffusivity around structured protein surfaces at equilibrium," *J. Am. Chem. Soc.* **139** (2017) 17890-17901.
DOI: 10.1021/jacs.7b08606
11. J.S. Bechtel, A. **Van der Ven**, "Octahedral tilting instabilities in inorganic halide perovskites," *Phys. Rev. Mater.* **2** (2018) 025401.
DOI: 10.1103/PhysRevMaterials.2.025401
12. M.F. Carilli, K.T. Delaney, G.H. **Fredrickson**, "Nucleation of the lamellar phase from the disordered phase of the renormalized Landau-Brazovskii model," *J. Chem. Phys.* **148** (2018) 054903.
DOI: 10.1063/1.5003150
13. W. Cheng, N. Singh, W. Elliott, J. Lee, A. Rassoolkhani, X. Jin, E. W. McFarland, S. Mubeen, "Earth-abundant tin sulfide-based photocathodes for solar hydrogen production," *Adv. Sci.* **5** (2018) 1700362.
DOI: 10.1002/advs.201700362
14. C. Cozzan, G. Lheureux, N. O'Dea, E.E. Levin, J. Graser, T.D. Sparks, S. Nakamura, S.P. DenBaars, C. Weisbuch, R. **Seshadri**, "Stable, heat-conducting phosphor composites for high-power laser lighting," *ACS Appl. Mater. Interfaces* **10** (2018) 5673-5681.
DOI: 10.1021/acsami.8b00074
15. S.P.O. Danielsen, G.E. Sanoja, S.R. McCuskey, B. Hammouda, G.C. Bazan, G.H. **Fredrickson**, R.A. **Segalman**, "Mixed conductive soft solids by electrostatically driven network formation of a conjugated polyelectrolyte," *Chem. Mater.* **30** (2018) 1417-1426.
DOI: 10.1021/acs.chemmater.7b05303
16. D.H. Fabini, T.A. Siaw, C.C. Stoumpos, G. Laurita, D. Olds, K. Page, J.G. Hu, M.G. Kanatzidis, S. **Han**, R. **Seshadri**, "Universal dynamics of molecular reorientation in hybrid lead iodide perovskites," *J. Am. Chem. Soc.* **139** (2017) 16875-16884.
DOI: 10.1021/jacs.7b09536
17. P. Ganguly, P. Boserma, N.F.A. van der Vegt, J.-E. **Shea**, "Trimethylamine *n*-oxide counteracts urea denaturation by inhibiting protein-urea preferential interaction," *J. Am. Chem. Soc.* **140** (2018) 483-492.
DOI: 10.1021/jacs.7b11695

18. M. Goyal, L. Galletti, S. Salmani-Rezaie, T. Schumann, D.A. Kealhofer, S. Stemmer, "Thickness dependence of the quantum Hall effect in films of the three-dimensional Dirac semimetal Cd_3As_2 ," *APL Mater.* **6** (2018) 026105.
DOI: 10.1063/1.5016866
19. J.H. Grebenkemper, J.D. Bocarsly, E.E. Levin, G. Seward, C. Heikes, C. Brown, S. Misra, F. Seeler, K. Schierle-Arndt, S.D. **Wilson**, R. **Seshadri**, "Rapid microwave preparation and composition tuning of the high-performance magnetocalorics $(\text{Mn,Fe})_2(\text{P,Si})$," *ACS Appl. Mater. Interfaces* **10** (2018) 7208-7213.
DOI: 10.1021/acsami.7b16988
20. Y. Kang, H. Peelaers, K. Krishnaswamy, C.G. **Van de Walle**, "First-principles study of direct and indirect optical absorption in BaSnO_3 ," *Appl. Phys. Lett.* **112** (2018) 062106.
DOI: 10.1063/1.5013641
21. N. Khalid, M. Hussain, H.S. Young, M. Ashraf, M. Hameed, R. Ahmad, "Lead concentrations in soils and some wild plant species along two busy roads in Pakistan," *Bull. Environ. Contam. Toxicol.* **100** (2018) 250-258.
DOI: 10.1007/s00128-017-2247-7
22. E. Lim, K.A. Peterson, G.M. Su, M.L. **Chabinyc**, "Thermoelectric properties of poly(3-hexylthiophene) (P3HT) doped with 2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F_4TCNQ) by vapor-phase infiltration," *Chem. Mater.* **30** (2018) 998-1010.
DOI: 10.1021/acs.chemmater.7b04849
23. J. Navarrete, C. Siefe, S. Alcantar, M. Belt, G.D. Stucky, M. Moskovits, "Merely measuring the UV-visible spectrum of gold nanoparticles can change their charge state," *Nano Lett.* **18** (2018) 669-674.
DOI: 10.1021/acs.nanolett.7b02592
24. R. Nery-Azevedo, A. Banerjee, T.M. **Squires**, "Diffusiophoresis in ionic surfactant gradients," *Langmuir* **33** (2017) 9694-9702.
DOI: 10.1021/acs.langmuir.7b01094
25. D.L. Poerschke, J.H. Shaw, N. Verma, F.W. Zok, C.G. Levi, "Interaction of yttrium disilicate environmental barrier coatings with calcium-magnesium-iron alumino-silicate melts," *Acta Mater.* **145** (2018) 451-461.
DOI: 10.1016/j.actamat.2017.12.004
26. M.B. Preefer, B. Oschmann, C. J. **Hawker**, R. **Seshadri**, F. Wudl, "High sulfur content material with stable cycling in lithium-sulfur batteries," *Angew. Chem. Int. Ed.* **56** (2017) 15118-15122.

DOI: 10.1002/anie.201708746

27. E.C. Schueller, G. Laurita, D.H. Fabini, C.C. Stoumpos, M.G. Kanatzidis, R. **Seshadri**, "Crystal structure evolution and notable thermal expansion in hybrid perovskites formamidinium tin iodide and formamidinium lead bromide," *Inorg. Chem.* **57** (2018) 695-701.
DOI: 10.1021/acs.inorgchem.7b02576
28. T. Schumann, L. Galletti, D.A. Kealhofer, H. Kim, M. Goyal, S. Stemmer, "Observation of the quantum hall effect in confined films of the three-dimensional Dirac semimetal Cd₃As₂," *Phys. Rev. Lett.* **120** (2018) 016801.
DOI: 10.1103/PhysRevLett.120.016801
29. S. Smeets, Z.J. Berkson, D. Xie, S.I. Zones, W. Wan, X. Zou, M.-F. Hsieh, B.F. **Chmelka**, L.B. McCusker, C. Baerlocher, "Well-defined silanols in the structure of the calcined high-silica zeolite SSZ-70: New understanding of a successful catalytic material," *J. Am. Chem. Soc.* **139** (2017) 16803-16812.
DOI: 10.1021/jacs.7b08810
30. D.C. Upham, V. Agarwal, A. Khechfe, Z.R. Snodgrass, M.J. Gordon, H. Metiu, E.W. McFarland, "Catalytic molten metals for the direct conversion of methane to hydrogen and separable carbon," *Science* **358** (2017) 917-921.
DOI: 10.1126/science.aao5023
31. N.R. Venkatesan, J.G. Labram, M.L. **Chabinyc**, "Charge-carrier dynamics and crystalline texture of layered Ruddlesden–Popper hybrid lead iodide perovskite thin films," *ACS Energy Lett.* **3** (2018) 380-386.
DOI: 10.1021/acsenergylett.7b01245
32. W. Wang; H. Peelaers; J.-X. Shen; A. Janotti; C.G. **Van de Walle**, "First-principles characterization of defects in WO₃," *Proceedings Vol. 10533, Oxide-based Materials and Devices IX*; 105332C (2018). Event: SPIE OPTO, 2018, San Francisco, CA.
DOI: 10.1117/12.2303688
33. M. Zhang, P.T. Corona, N. Ruocco, D. Alvarez, P. Malo de Molina, S. Mitragotri, M.E. **Helgeson**, "Controlling complex nanoemulsion morphology using asymmetric cosurfactants for the preparation of polymer nanocapsules," *Langmuir* **34** (2018) 978-990.
DOI: 10.1021/acs.langmuir.7b02843