

Hydrogen Materials Advanced Research Consortium (HyMARC) Publications

2022

Allendorf, M.D., V. Stavila, J. L. Snider, M. Witman, M. E. Bowden, K. Brooks, B. L. Tran, and T. Autrey. "Challenges to developing materials for the transport and storage of hydrogen" *Nat. Chem.* (2022) <https://doi.org/10.1038/s41557-022-01056-2>

Correll, H., N Leick, RE Mow, GA Russell-Parks, SH Pang, T Gennett, "Fluorescent Probe of Aminopolymer Mobility in Bulk and in Nanoconfined Direct Air CO₂ Capture Supports." *The Journal of Physical Chemistry C* 126 (25), 10419-10428 (2022) <https://doi.org/10.1021/acs.jpcc.2c01099>

Densified HKUST-1 Monoliths as a Route to High Volumetric and Gravimetric Hydrogen Storage Capacity DG Madden, D O'Nolan, N Rampal, R Babu, C Çamur, AN Al Shakhs, et.al. *J. Am. Chem. Soc.* 2022, 144, 30, 13729–13739

Photo triggered covalent organic frameworks and methods of using DR Vardon, WA Braunecker, JC Johnson, T Gennett, RE Mow, US Patent App. 17/393,961, 2022

Reversible dehydrogenation and rehydrogenation of cyclohexane and methylcyclohexane by single-site platinum catalyst, L Chen, P Verma, K Hou, Z Qi, S Zhang, YS Liu, J Guo, V Stavila, *Nature communications* 13 (1), 1-9, 2022

Reactive Vapor-Phase Additives toward Destabilizing γ -Mg(BH₄)₂ for Improved Hydrogen Release NA Strange, N Leick, S Shulda, A Schneemann, V Stavila, AS Lipton, ..., *ACS Applied Energy Materials* 5 (2), 1690-1700

Thermal stability and structural studies on the mixtures of Mg (BH₄)₂ and glymes N Leick, BL Tran, ME Bowden, T Gennett, T Autrey *Dalton Transactions* 51 (18), 7268-7273, 2022

Cost and potential of metal-organic frameworks for hydrogen back-up power supply, P Peng, A Anastasopoulou, K Brooks, H Furukawa, ME Bowden, JR Long, *Nature Energy* 7 (5), 448-458, 1, 2022

Research and development of hydrogen carrier based solutions for hydrogen compression and storage, M Dornheim, L Baetcke, E Akiba, JR Ares, T Autrey, J Barale, M Baricco, et. Al, *Prog. Energy* 4, 042005, 2022

Hydrogen storage in complex hydrides: past activities and new trends, EMM Dematteis, MB Amdisen, T Autrey, J Barale, M Bowden, CE Buckley, ..., *Progress in Energy*, 2022

First-Principles Elucidation of Initial Dehydrogenation Pathways in Mg(BH₄)₂, LF Wan, T Autrey, BC Wood, *The Journal of Physical Chemistry Letters* 13 (8), 1908-1913, 2022

12. Analysis of Intermediates and Products from the Dehydrogenation of Mg(BH₄)₂, IH Nayyar, B Ginovska, M Bowden, G Edvenson, B Tran, T Autrey, *The Journal of Physical Chemistry A* 126 (3), 444-452, 3, 2022

Thermal stability and structural studies on the mixtures of Mg (BH₄)₂ and glymes, N Leick, BL Tran, ME Bowden, T Gennett, T Autrey, *Dalton Transactions* 51 (18), 7268-7273

Hydrogen Storage Performance of Preferentially Oriented Mg/rGO Hybrids, C Dun, S Jeong, DH Kwon, SY Kang, V Stavila, Z Zhang, JW Lee, B. C. Wood, Chemistry of Materials 34 (7), 2963-2971

Heteroatom-Doped Graphenes as Actively Interacting 2D Encapsulation Media for Mg-Based Hydrogen Storage, YJ Cho, SY Kang, BC Wood, ES Cho, ACS Appl. Mater. Interfaces 2022, 14, 18, 20823–20834

Magnesium-and intermetallic alloys-based hydrides for energy storage: modelling, synthesis and properties, L Pasquini, K Sakaki, E Akiba, MD Allendorf, E Alvares, JR Ares, D Babai Progress in Energy 4 (3), 032007

Vanadium metal-organic framework for selective adsorption, JR Long, DE Jaramillo, DA Reed US Patent 11,311,856, 2022

Understanding Hydrogenation Chemistry at MgB₂ Reactive Edges from Ab Initio Molecular Dynamics, KG Ray, LE Klebanoff, V Stavila, SY Kang, LF Wan, S Li, TW Heo, et. Al, ACS ACS Appl. Mater. Interfaces 2022, 14, 18, 20430–20442

Reversible dehydrogenation and rehydrogenation of cyclohexane and methylcyclohexane by single-site platinum catalyst, L Chen, P Verma, K Hou, Z Qi, S Zhang, YS Liu, J Guo, V Stavila, et. Al, Nature communications 13 (1), 1-9, 5, 2022

The influence of LiH and TiH₂ on hydrogen storage in MgB₂ II. XPS study of surface and near-surface phenomena, JL Snider, TM Mattox, YS Liu, LF Wan, P Wijeratne, MD Allendorf, International Journal of Hydrogen Energy 47 (1), 403-419

Reveal the Alignment of Defects in a Metal-Organic Framework with Tunable Flexibility, Y Fu, A Forse, Z Kang, M Cliffe, W Cao, J Yin, L Gao, Z Pang, T He, .et.al, Research Square, 2022

“Thermal conversion of unsolvated Mg(B₃H₈)₂ to BH₄⁻ in the presence of MgH₂” A. Gigante, N. Leick, A. Lipton, B. Tran, N. Strange, M. Bowden, M. Martinez, R. Moury, T. Gennett, H. Hagemann, T. Autrey, ACS Applied Energy Materials in press (2021)

“Stabilized Open Metal Sites in Bimetallic Metal-Organic Framework Catalysts for Hydrogen Production” J. L. Snider, J. Su, P. Verma, F. El Gabaly, J. D. Sugar, L. Chen, J. M. Chames, A. A. Talin, C. Dun, J. J. Urban, V. Stavila, D. Prendergast, G. A. Somorjai, M. D. Allendorf J. Mater. Chem. A 2021, DOI: 10.1039/D1TA00222H.

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“Al₂O₃ Atomic Layer Deposition on nanostructured γ -Mg(BH₄)₂ for H₂ storage” N. Leick, N. Strange, A. Schneemann, V. Stavila, K. Gross, N. Washton, A. Settle, M. Martinez, T. Gennett, S. Christensen, ACS Applied Energy Materials 4, 2, 1150 (2021)

“Heterolytic Scission of Hydrogen Within a Crystalline Frustrated Lewis Pair” M. Bowden, B. Ginovska, M. Jones, A. Karkamkar, A. Rameriz Cuesta, L. Daemen, G. Schenter, S. Miller, T. Repo, K. Chernichenko, N. Leick, M. Martinez, T. Autrey, Inorg. Chem. 59, 20, 15295 (2020)

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J. L. White; A. A. Baker; M. A. Marcus; J. L. Snider; T. C. Wang; J. R. I. Lee; D. A. L. Kilcoyne; M. D. Allendorf; V. Stavila; F. El Gabaly "The Inside-Outs of Metal Hydride Dehydrogenation: Imaging the Phase Evolution of the Li-N-H Hydrogen Storage System," *Advanced Materials Interfaces* 2020, 7, 1901905.

J. L. White; N. A. Strange; J. D. Sugar; J. L. Snider; A. Schneemann; A. S. Lipton; M. F. Toney; M. D. Allendorf; V. Stavila "Melting of Magnesium Borohydride under High Hydrogen Pressure: Thermodynamic Stability and Effects of Nanoconfinement," *Chemistry of Materials* 2020, 32, 5604.

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“Statistically-Averaged Molecular Dynamics Simulations of Hydrogen Diffusion in Magnesium and Magnesium Hydrides,” C. Spataru, T. W. Heo, B. C. Wood, V. Stavila, S. Kang, M. Allendorf, and X. Zhou, Phys. Rev. Mater., 4, 105401 (2020)

“Nanoscale Mg-B Via Surfactant Ball Milling of MgB₂: Morphology, Composition and Improved Hydrogen Storage Properties”, Y.-S. Liu, K. Ray, M. Jørgensen, T. Mattox, D. Cowgill, H. Eshelman, A. Sawvel, J. Snider, W. York, P. Wijeratne, A. Pham, G. Harini, S. Li, T. W. Heo, S. Kang, T. Jensen, V. Stavila, B. Wood, and L. Klebanoff, J. Phys. Chem C., 124, 21761 (2020)

“Beyond idealized models of nanoscale metal hydrides for hydrogen storage”, B.C. Wood, T.W. Heo, S. Kang, L.F. Wan, and S. Li, Industrial & Engineering Chem. Res., 59, 5786 (2020)

Catalytic Hydrogen Production from Methane: A Review on Recent Progress and Prospect. L. N. Chen, Z. Y. Qi, S. C. Zhang, J. Su, G. A. Somorjai, Catalysis 10, 858 (2020).

Nanoconfinement of Molecular Magnesium Borohydride Captured in a Bipyridine-Functionalized Metal-Organic Framework A. Schneemann, L. F. Wan, A. S. Lipton, Y. S. Liu, J. L. Snider, A. A. Baker, J. D. Sugar, C. D. Spataru, J. H. Guo, T. S. Autrey, M. Jørgensen, T. R. Jensen, B. C. Wood, M. D. Allendorf, V. Stavila, ACS Nano 14, 10294 (2020).

Calcium chloride substitution in sodium borohydride. T. M. Mattox, G. Bolek, A. L. Pham, M. Kunz, Y. S. Liu, S. C. Fakra, M. P. Gordon, A. Doran, J. H. Guo, J. J. Urban, J Sol Stat Chem 290, 121499 (2020).

“Interplay of NH₄⁺ and BH₄⁺ Reorientational Dynamics in NH₄BH₄,” M. S. Andersson, J. B. Grinderslev, T. R. Jensen, V. García Sakai, U. Häussermann, T. J. Udovic, and M. Karlsson, Phys. Rev. Materials 4, 085002 (2020).

“Na⁺ Diffusivity in Carbon-Substituted nido- and closo-Hydroborate Salts: Pulsed-Field-Gradient NMR Studies of Na-7-CB₁₀H₁₃ and Na₂(CB₉H₁₀)(CB₁₁H₁₂),” A. V. Skripov, G. Majer, O. A. Babanova, R. V. Skoryunov, A. V. Soloninin, M. Dimitrievska, and T. J. Udovic, J. Alloys Compd. 850, 156781 (2021).

“Interplay Between the Reorientational Dynamics of the B₃H₈⁻ Anion and the Structure in KB₃H₈,” M. S. Andersson, J. B. Grinderslev, X.-M. Chen, X. Chen, U. Häussermann, W. Zhou, T. R. Jensen, M. Karlsson, and T. J. Udovic, J. Phys. Chem. C 125, 3716-3724 (2021).

“Lithium-Ion Diffusivity in Complex Hydrides: Pulsed-Field-Gradient NMR Studies of $\text{LiLa}(\text{BH}_4)_3\text{Cl}$, $\text{Li}_3(\text{NH}_2)_2\text{I}$ and Li-1-CB9H_{10} ,” A. V. Skripov, G. Majer, O. A. Babanova, R. V. Skoryunov, A. V. Soloninin, M. B. Ley, T. R. Jensen, S. Orimo, and T. J. Udovic, *Solid State Ionics* 362, 115585 (2021).

“Design Principles for the Ultimate Gas Deliverable Capacity Material: Nonporous to Porous Deformations without Volume Change” Witman, M.; Ling, S.; Stavila, V.; Wijeratne, P.; Furukawa, H.; Allendorf, M. D. *Mol. Syst. Des. Eng.* 2020, 5, 1491–1503

"Extracting an Empirical Intermetallic Hydride Design Principle from Limited Data Via Interpretable Machine Learning," M. Witman; S. L. Ling; D. M. Grant; G. S. Walker; S. Agarwal; V. Stavila; M. D. Allendorf *Journal of Physical Chemistry Letters* 2020, 11, 40.

“Ambient-Temperature Hydrogen Storage via Vanadium(II)-Dihydrogen Complexation in a Metal–Organic Framework” Jaramillo, D. E.; Jiang, H. Z. H.; Evans, H. A.; Chakraborty, R.; Furukawa, H.; Brown, C. M.; Head-Gordon, M.; Long, J. R. *J. Am. Chem. Soc.* 2021, 143, in press.

“Structural and Dynamical Properties of Potassium Dodecahydro-Monocarba-Closo-Dodecaborate: $\text{KCB}_{11}\text{H}_{12}$,” M. Dimitrievska, H. Wu, V. Stavila, O. A. Babanova, R. V. Skoryunov, A. V. Soloninin, W. Zhou, B. A. Trump, M. S. Andersson, A. V. Skripov, and T. J. Udovic, *J. Phys. Chem. C* 124, 17992-18002 (2020).

“Chemical Bonding Governs Complex Magnetism in MnPt_5P .” Gui, X.; Klein, R. A.; Brown, C. M.; Xie, W. *Inorganic Chemistry* 2021, 60, 87–96.

Predicting Hydrogen Storage in MOFs via Machine Learning Ahmed, Alauddin; Siegel, Donald (2020): *ChemRxiv*. Preprint. <https://doi.org/10.26434/chemrxiv.13345250.v1>

A Mechanistic Analysis of Phase Evolution and Hydrogen Storage Behavior in Nanocrystalline $\text{Mg}(\text{BH}_4)_2$ within Reduced Graphene Oxide

Nanoscale Mg-B via Surfactant Ball Milling of MgB_2 : Morphology, Composition, and Improved Hydrogen Storage Properties Y. S. Liu, K. G. Ray, M. Jorgensen, T. M. Mattox, D. F. Cowgill, H. V. Eshelman, A. M. Sawvel, J. L. Snider, W. York, P. Wijeratne, A. L. Pham, H. Gunda, S. Li, T. W. Heo, S. Kang, T. R. Jensen, V. Stavila, B. C. Wood, L. E. Klebanoff, *J Phys Chem C* 124, 21761 (2020)

Phonon Dispersion Relation of Bulk Boron-Doped Graphitic Carbon. D. McGlamery, A. A. Baker, Y. S. Liu, M. A. Mosquera, N. P. Stadie, *J. Phys Chem C* 124, 23027 (2020)

Enhanced and stabilized hydrogen production from methanol by ultrasmall Ni nanoclusters immobilized on defect-rich h-BN nanosheets. Z. Zhang, J. Su, A. Sanz Matias, M. Gordon, Y. S. Liu, J. Guo, C. Song, C. Dun, D. Prendergast, G. A. Somorjai, J. J. Urban, *Proc. Nat. Acad. Sci.* 117, 29442 (2020)

Colloidal Three-Dimensional Covalent Organic Frameworks and Their Application as Porous Liquids R. E. Mow, A. S. Lipton, S. Shulda, E. A. Gauding, T. Gennett, W. A. Braunecker,* , *J. Mater. Chem. A.*, 2020, 8, 23455-23462

2021

A. Gigante, N. Leick, A. Lipton, B. Tran, N. Strange, M. Bowden, M. Martinez, R. Moury, T. Gennett, H. Hagemann, T. Autrey, "Thermal conversion of unsolvated $Mg(B3H8)_2$ to BH_4^- in the presence of MgH_2 " ACS Applied Energy eMaterials in press (2021)

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C. D. Spataru, J. H. Guo, T. S. Autrey, M. Jorgensen, T. R. Jensen, B. C. Wood, M. D. Allendorf, V. Stavila, ACS Nano 14, 10294 (2020).

"Na⁺ Diffusivity in Carbon-Substituted nido- and closo-Hydroborate Salts: Pulsed-Field-Gradient NMR Studies of Na-7-CB10H13 and Na₂(CB9H10)(CB11H12)," A. V. Skripov, G. Majer, O. A. Babanova, R. V. Skoryunov, A. V. Soloninin, M. Dimitrievska, and T. J. Udovic, J. Alloys Compd. 850, 156781 (2021).

"Interplay Between the Reorientational Dynamics of the B₃H₈⁻ Anion and the Structure in KB₃H₈," M. S. Andersson, J. B. Grinderslev, X.-M. Chen, X. Chen, U. Häussermann, W. Zhou, T. R. Jensen, M. Karlsson, and T. J. Udovic, J. Phys. Chem. C 125, 3716-3724 (2021).

"Lithium-Ion Diffusivity in Complex Hydrides: Pulsed-Field-Gradient NMR Studies of LiLa(BH₄)₃Cl, Li₃(NH₂)₂I and Li-1-CB₉H₁₀," A. V. Skripov, G. Majer, O. A. Babanova, R. V. Skoryunov, A. V. Soloninin, M. B. Ley, T. R. Jensen, S. Orimo, and T. J. Udovic, Solid State Ionics 362, 115585 (2021).

"Design Principles for the Ultimate Gas Deliverable Capacity Material: Nonporous to Porous Deformations without Volume Change" Witman, M.; Ling, S.; Stavila, V.; Wijeratne, P.; Furukawa, H.; Allendorf, M. D. Mol. Syst. Des. Eng. 2020, 5, 1491–1503

"Extracting an Empirical Intermetallic Hydride Design Principle from Limited Data Via Interpretable Machine Learning," M. Witman; S. L. Ling; D. M. Grant; G. S. Walker; S. Agarwal; V. Stavila; M. D. Allendorf Journal of Physical Chemistry Letters 2020, 11, 40.

"Ambient-Temperature Hydrogen Storage via Vanadium(II)-Dihydrogen Complexation in a Metal–Organic Framework" Jaramillo, D. E.; Jiang, H. Z. H.; Evans, H. A.; Chakraborty, R.; Furukawa, H.; Brown, C. M.; Head-Gordon, M.; Long, J. R. J. Am. Chem. Soc. 2021, 143, in press.

"Structural and Dynamical Properties of Potassium Dodecahydro-Monocarba-Closo-Dodecaborate: KCB₁₁H₁₂," M. Dimitrievska, H. Wu, V. Stavila, O. A. Babanova, R. V. Skoryunov, A. V. Soloninin, W. Zhou, B. A. Trump, M. S. Andersson, A. V. Skripov, and T. J. Udovic, J. Phys. Chem. C 124, 17992-18002 (2020).

"Chemical Bonding Governs Complex Magnetism in MnPt₅P." Gui, X.; Klein, R. A.; Brown, C. M.; Xie, W. Inorganic Chemistry 2021, 60, 87–96.

Predicting Hydrogen Storage in MOFs via Machine Learning Ahmed, Alauddin; Siegel, Donald (2020): ChemRxiv. Preprint. <https://doi.org/10.26434/chemrxiv.13345250.v1>

"A Mechanistic Analysis of Phase Evolution and Hydrogen Storage Behavior in Nanocrystalline Mg(BH₄)₂ within Reduced Graphene Oxide."

"Nanoscale Mg-B via Surfactant Ball Milling of MgB₂: Morphology, Composition, and Improved Hydrogen Storage Properties." Y. S. Liu, K. G. Ray, M. Jorgensen, T. M. Mattox, D. F. Cowgill, H. V. Eshelman, A. M. Sawvel, J. L. Snider, W. York, P. Wijeratne, A. L. Pham, H. Gunda, S. Li, T. W. Heo, S. Kang, T. R. Jensen, V. Stavila, B. C. Wood, L. E. Klebanoff, J Phys Chem C 124, 21761 (2020)

"Phonon Dispersion Relation of Bulk Boron-Doped Graphitic Carbon. D. McGlamery." A. A. Baker, Y. S. Liu, M. A. Mosquera, N. P. Stadie, J. Phys Chem C 124, 23027 (2020)

Zhang, Z., J. Su, A. Sanz Matias, M. Gordon, Y. S Liu, J. Guo, C. Song, C. Dun, D. Prendergast, G. A. Somorjai, and J. J. Urban. "Enhanced and stabilized hydrogen production from methanol by ultrasmall Ni nanoclusters immobilized on defect-rich h-BN nanosheets." *Proc. Nat. Acad. Sci.* 117 (2020): 29442

Mow, R. E., A. S. Lipton, S. Shulda, E. A. Gaulding, T. Gennett, and W. A. Braunecker. "Colloidal Three-Dimensional Covalent Organic Frameworks and Their Application as Porous Liquids." *J. Mater. Chem. A.*, 8 (2020): 23455-23462

2020

Biggins, N., M. E. Ziebel, M. I. Gonzalez, and J. R. Long. "Crystallographic Characterisation of Reductive Cation Insertion into the Metal–Organic Framework $\text{Fe}_2(\text{bdp})_3$." *Chem. Sci.* 11 (2020): 9173–9180. <https://doi.org/10.1039/d0sc03383a>.

Braunecker, W. A., S. Shulda, M. B. Martinez, K. E. Hurst, J. T. Koubek, S. Zaccarine, R. E. Mow, S. Pylypenko, A. Sellinger, T. Gennett, and J. C. Johnson. "Thermal Activation of a Copper-Loaded Covalent Organic Framework for Near-Ambient Temperature Hydrogen Storage and Delivery." *ACS Materials Lett.* 2, no. 3 (2020): 227–232.

Dimitrievska, M., M. Chong, M. E. Bowden, H. Wu, W. Zhou, I. Nayyar, B. Ginovska, T. Gennett, T. Autrey, C. M. Jensen, and T. J. Udovic. "Solvent Addition as a Solution for Enhancing Hydrogen Storage Properties of Magnesium-Borohydride." *Phys. Chem. Chem. Phys.* 22 (2020): 368–378. <https://doi.org/10.1039/C9CP03311D>.

Grubel K., H. Jeong, C. Yoon, and T. Autrey. "Challenges and Opportunities for Using Formate to Store, Transport and Utilize Hydrogen." *Journal of Energy Chemistry* 41 (2020): <https://doi.org/10.1016/j.jechem.2019.05.016>.

Grubel, K., J. Su, J. Kothandaraman, K. Brooks, G. A. Somorjai, and T. Autrey. "Research Requirements to Move the Bar Forward Using Aqueous Formate Salts as H_2 Carriers for Energy Storage Applications." Invited perspective. *Journal of Energy and Technology* (2020).

Halter, D. P., R. A. Klein, M. A. Boreen, B. A. Trump, C. M. Brown, and J. R. Long. "Self-Adjusting Binding Pockets Enhance H_2 and CH_4 Adsorption in a Uranium-Based Metal–Organic Framework." *Chem. Sci.* 11 (2020): 6709–6716. <https://doi.org/10.1039/D0SC02394A>.

Hwang, Y. J., Y. Kwon, Y. Kim, H. Sohn, S. W. Nam, J. Kim, T. Autrey, C. W. Yoon, Y. S. Jo, and H. Jeong. "Development of an Autothermal Formate-Based Hydrogen Generator: From Optimization of Formate Dehydrogenation Conditions to Thermal Integration with Fuel Cells." *ACS Sustainable Chem. Eng.* 8, no. 26 (2020): 9846. <https://doi.org/10.1021/acssuschemeng.0c02775>.

Jaramillo, D. E., D. A. Reed, H. Z. H. Jiang, J. Oktawiec, M. W. Mara, A. C. Forse, D. J. Lussier, R. A. Murphy, M. Cunningham, V. Colombo, D. K. Shuh, J. A. Reimer, and J. R. Long. "Selective Nitrogen Adsorption via Backbonding in a Metal–Organic Framework with Exposed Vanadium Sites." *Nature Mater.* 19 (2020): 517–521. <https://doi.org/10.1038/s41563-019-0597-8>.

Jeong, S., T. W. Heo, J. Oktawiec, R. Shi, S. Kang, J. L. White, A. Schneemann, E. W. Zaia, L. F. Wan, K. G. Ray, Y.-S. Liu, V. Stavila, J. Guo, J. R. Long, B. C. Wood, and J. J. Urban. "A Mechanistic Analysis of Phase

Evolution and Hydrogen Storage Behavior in Nanocrystalline $\text{Mg}(\text{BH}_4)_2$ within Reduced Graphene Oxide.” *ACS Nano* 14, no. 2 (2020): 1745–1756.

Jørgensen, M., P. T. Shea, A. W. Tomich, J. B. Varley, M. Bercx, S. Lovera, R. Černý, W. Zhou, T. J. Udovic, V. Lavallo, T. R. Jensen, B. C. Wood, and V. Stavila. “Understanding Superionic Conductivity in Lithium and Sodium Salts of Weakly Coordinating Closo-Hexahalocarborate Anions.” *Chem. Mater.* 32, no. 4 (2020): 1475–1487.

Liu, Y. S., K. G. Ray, M. Jorgensen, T. M. Mattox, D. F. Cowgill, H. V. Eshelman, A. M. Sawvel, J. L. Snyder, W. York, P. Wijeratne, A. L. Pham, H. Gunda, S. Li, T. W. Heo, S. Kang, T. R. Jensen, V. Stavila, B. C. Wood, and L. E. Klebanoff. “Nanoscale Mg–B via Surfactant Ball Milling of MgB_2 : Morphology, Composition and Improved Hydrogen Storage Properties.” *J. Phys. Chem. C* 124, no. 39 (2020): 21761–21771.

<https://doi.org/10.1021/acs.jpcc.0c05142>.

Nayyar, I. H., B. Ginovska, A. Karkamkar, T. Gennett, and T. Autrey. “Physi-Sorption of H_2 on Pure and Boron–Doped Graphene Monolayers: A Dispersion–Corrected DFT Study.” Invited Special Issue Carbon-Based Materials for Hydrogen Production, Storage and Conversion. *C Journal of Carbon Research* (2020). <https://doi.org/10.3390/c6010015>. PNNL-SA-150699.

Schneemann, A., L. F. Wan, A. S. Lipton, Y.-S. Liu, J. L. Snider, A. A. Baker, J. D. Sugar, C. D. Spataru, J. Guo, T. S. Autrey, M. Jørgensen, T. R. Jensen, B. C. Wood, M. D. Allendorf, and V. Stavila.

“Nanoconfinement of Molecular Magnesium Borohydride Captured in a Bipyridine-Functionalized Metal–Organic Framework.” *ACS Nano* 14, no. 8 (2020): 10294–10304.

<https://doi.org/10.1021/acsnano.0c03764>.

Spataru, C. D., T. W. Heo, B. C. Wood, V. Stavila, S. Kang, M. D. Allendorf, and X. W. Zhou. “Statistically Averaged Molecular Dynamics Simulations of Hydrogen Diffusion in Magnesium and Magnesium Hydrides.” *Phys. Rev. Materials* 4 (2020): 105401. <https://doi.org/10.1103/PhysRevMaterials.4.105401>.

Taylor, M. K., M. Juhl, G. B. Hadaf, D. Hwang, E. Velasquez, J. Oktawiec, J. B. Lefton, T. Runčevski, J.R. Long, and J.-W. Lee. “Palladium-Catalyzed Oxidative Homocoupling of Pyrazole Boronic Esters to Access Versatile Bipyrazoles and the Flexible Metal–Organic Framework $\text{Co}(4,4'\text{-bipyrazolate})$.” *Chem. Commun.* 56 (2020): 1195–1198. <https://doi.org/10.1039/c9cc08614e>.

Veccham, S. R., and M. Head-Gordon. “Density Functionals for Hydrogen Storage: Defining the $\text{H}_2\text{Bind}275$ Test Set with ab initio Benchmarks and Assessment of 55 Functionals.” *J. Chem. Theory Comput.* 16 (2020): 4963–4982. <https://doi.org/10.1021/acs.jctc.0c00292>.

White, J. L., A. A. Baker, M. A. Marcus, J. L. Snider, T. C. Wang, J. R. Lee, D. A. L. Kilcoyne, M. D. Allendorf, V. Stavila, and F. El Gabaly. “The Inside-Outs of Metal Hydride Dehydrogenation: Imaging the Phase Evolution of the Li–N–H Hydrogen Storage System.” *Adv. Mater. Interfaces* 7 (2020): 1901905. <https://doi.org/10.1002/admi.201901905>.

White, J. L., N. A. Strange, J. D. Sugar, J. L. Snider, A. Schneemann, A. S. Lipton, M. F. Toney, M. D. Allendorf, and V. Stavila. “Melting of Magnesium Borohydride under High Hydrogen Pressure: Thermodynamic Stability and Effects of Nanoconfinement.” *Chem. Mater.* 32 (2020): 5604.

<https://doi.org/10.1021/acs.chemmater.0c01050>.

Witman, M., S. L. Ling, D. M. Grant, G. S. Walker, S. Agarwal, V. Stavila, and M. D. Allendorf. "Extracting an Empirical Intermetallic Hydride Design Principle from Limited Data via Interpretable Machine Learning." *J. Phys. Chem. Lett.* 11 (2020): 40. <https://doi.org/10.1021/acs.jpcllett.9b02971>.

Witman, M., S. Ling, V. Stavila, P. Wijeratne, H. Furukawa, and M. D. Allendorf. "Design Principles for the Ultimate Gas Deliverable Capacity Material: Nonporous to Porous Deformations without Volume Change." *Mol. Syst. Des. Eng.* 5 (2020): 1491. <https://doi.org/10.1039/d0me00122h>.

Wood, B. C., T. W. Heo, S. Kang, S. Li, and L. F. Wan. "Beyond Idealized Models of Nanoscale Metal Hydrides for Hydrogen Storage." Invited article. *Ind. Eng. Chem. Res.* 59 (2020): 5786–5796.

2019

Chen, L., K. Hou, Y.-S. Liu, Zh. Qi, Q. Zheng, Y. Lu, J. Chen, J. Chen, Ch. Pao, Sh. Wang, Y. Li, Sh. Xie, F. Liu, D. Prendergast, L. Klebanoff, V. Stavila, M. Allendorf, J.-H. Guo, L. Zheng, J. Su, and A. G. Somorjai. "Efficient Hydrogen Production from Methanol Using A Single-Site Pt₁/CeO₂ Catalyst." *J. Amer. Chem. Soc.* 141, no. 45 (2019): 17995–17999. <https://doi.org/10.1021/jacs.9b09431>.

Grubel, K., H. Jeong, C. W. Yoon, and T. Autrey. "Challenges and Opportunities for Using Formate to Store, Transport, and Use Hydrogen." *J. Energy Chemistry* (2019). <https://doi.org/10.1016/j.jechem.2019.05.016>.

Heo, T. W., K. B. Colas, A. T. Motta, and L.-Q. Chen. "A Phase-Field Model for Hydride Formation in Polycrystalline Metals: Application to δ -Hydride in Zirconium Alloys." *Acta Mater.* 181 (2019): 262.

Heo, T. W., and B.C. Wood. "On Thermodynamic and Kinetic Mechanisms for Stabilizing Surface Solid Solutions." *ACS Appl. Mater. Interf.* 11 (2019): 48487.

Hirscher, M., T. Autrey, and S. Orimo. "Hydrogen Energy." Invited. *ChemPhysChem* 20, no. 10 (2019): 1157. <https://doi.org/10.1002/cphc.201900429>. PNNL-SA-143944.

Hong, W., M. Kitta, N. Tsumori, Y. Himeda, T. Autrey, and Q. Xu. "Immobilization of Highly Active Bimetallic PdAu Nanoparticles to Nanocarbons for Dehydrogenation of Formic Acid." *Journal of Materials Chemistry A* (2019). <https://doi.org/10.1039/C9TA06014F>. TA-COM-06-2019-006014.R1.

Hurst, K. E., T. Gennett, J. Adams, M. D. Allendorf, R. Balderas-Xicohtencatl, M. Bielewski, B. Edwards, L. Espinal, B. Fultz, M. Hirscher, M. S. L. Hudson, Z. Hulvey, M. Latroche, D. J. Liu, M. Kapelewski, E. Napolitano, Z. T. Perry, J. Purewal, V. Stavila, M. Veenstra, J. L. White, Y. P. Yuan, H. C. Zhou, C. Zlotea, and P. Parilla. "An International Laboratory Comparison Study of Volumetric and Gravimetric Hydrogen Adsorption Measurements." *ChemPhysChem* 20 (2019): 1997. <https://doi.org/10.1002/cphc.201900166>.

Jeong, S., P. Milner, L. F. Wan, Y.-S. Liu, J. Oktawiec, E. W. Zaia, J.-H. Guo, D. Prendergast, J. R. Long, and J. J. Urban. "Runaway Carbon Dioxide Conversion Leads to Enhanced Sorption in a Nanohybrid Porous Magnesium Metal Hydride." *Advanced Materials* 31, no. 44 (2019): e1904252. <https://doi.org/10.1002/adma.201904252>. Work highlighted in C&E News.

Kang, S., T. W. Heo, M. D. Allendorf, and B. C. Wood. "Morphology-Dependent Stability of Complex Metal Hydrides and Their Intermediates Using First-Principles Calculations." *ChemPhysChem* 20 (2019): 1340. <https://doi.org/10.1002/cphc.201801132>.

Kumar, R., A. Karkamkar, M. Bowden, and T. Autrey. "Boron-Nitrogen Containing Compounds in Energy Storage." Invited. *Chem. Soc. Rev.* 48 (2019): 5350. <https://doi.org/10.1039/C9CS00442D>. PNNL-SA-146182.

Liu, Y. S., S. Jeong, J. L. White, X. F. Feng, E. S. Cho, V. Stavila, M. D. Allendorf, J. J. Urban, and J. H. Guo. "In-Situ/Operando X-Ray Characterization of Metal Hydrides." *ChemPhysChem* 20 (2019): 1261. <https://doi.org/10.1002/cphc.201801185>.

Liu, Y.-S., L. E. Klebanoff, P. Wijeratne, D. F. Cowgill, V. Stavila, T. W. Heo, S. Kang, A. A. Baker, J. R. I. Lee, K. G. Ray, J. D. Sugar, and B. C. Wood. "Investigating Possible Kinetic Limitations to MgB₂ Hydrogenation." *Int. J. Hydrogen Energy* 44 (2019): 31239. <https://doi.org/10.1016/j.ijhydene.2019.09.125>.

Stauch, T., R. Chakraborty, and M. Head-Gordon. "Quantum Chemical Modeling of Pressure-Induced Spin Crossover in Octahedral Metal-Ligand Complexes." *ChemPhysChem* 20 (2019): 2742.

Stavila, V., M. E. Foster, J. W. Brown, R. W. Davis, J. Edgington, A. I. Benin, R. A. Zarkesh, R. Parthasarathi, D. W. Hoyt, E. D. Walter, A. Andersen, N. M. Washton, A. S. Lipton, and M. D. Allendorf. "IRMOF-74(n)-Mg: A Novel Catalyst Series for Hydrogen Activation and Hydrogenolysis of C-O Bonds." *Chem. Sci.* 10 (2019): 9880. <https://doi.org/10.1039/c9sc01018a>.

Sugai, C., S. Kim, G. Severa, J. L. White, N. Leick, M. B. Martinez, T. Gennett, V. Stavila, and C. Jensen. "Kinetic Enhancement of Direct Hydrogenation of MgB₂ to Mg(BH₄)₂ upon Mechanical Milling with THF, MgH₂, and/or Mg." *ChemPhysChem* 10 (2019): 1301.

Tsumori, N., Y. Himeda, T. Autrey, and Q. Xu. "Immobilization of Highly Active Bimetallic PdAu Nanoparticles onto Nanocarbons for Dehydrogenation of Formic Acid." *Journal of Materials Chemistry A* 7, no. 32 (2019): 18835–18839. <https://doi.org/10.1039/c9ta06014f>. PNNL-SA-148310.

Wan, L. F., E. S. Cho, T. Marangoni, P. Shea, S. Y. Kang, C. Rogers, E. Zaia, R. R. Cloke, B. C. Wood, F. R. Fischer, J. J. Urban, and D. Prendergast. "Edge-Functionalized Graphene Nanoribbon Encapsulation to Enhance Stability and Control Kinetics of Hydrogen Storage Materials." *Chem. Mater.* 31, no. 8 (2019): 2960–2970. <https://doi.org/10.1021/acs.chemmater.9b00494>.

Wang, T. C., J. L. White, B. L. Bie, H. X. Deng, J. Edgington, J. D. Sugar, V. Stavila, and M. D. Allendorf. "Design Rules for Metal-Organic Framework Stability in High-Pressure Hydrogen Environments." *ChemPhysChem* 20 (2019): 1305. <https://doi.org/10.1002/cphc.201801190>.

White, J. L., A. J. E. Rowberg, L. F. Wan, S. Y. Kang, T. Ogitsu, R. D. Kolasinski, J. A. Whaley, A. Baker, J. R. I. Lee, Y. S. Liu, L. Trotochaud, J.-H. Guo, V. Stavila, D. Prendergast, H. Bluhm, M. D. Allendorf, B. C. Wood, and F. E. Gabaly. "Identifying the Role of Dynamic Surface Hydroxides in the Dehydrogenation of Ti-doped NaAlH₄." *ACS Appl. Mater. Interfaces* 11 (2019): 4930–4941. <https://doi.org/10.1021/acsami.8b17650>.

Yu, Y., T. He, A. Wu, Q. Pei, A. J. Karkamkar, T. Autrey, and P. Chen. "Reversible Hydrogen Uptake/Release over Sodium Phenoxide-Cyclohexanolate Pair." *Angewandte Chemie International Edition* 58, no. 10 (2019): 3102–3107. <https://doi.org/10.1002/anie.201810945>.

Zhou, X. W., S. Kang, T. W. Heo, B. C. Wood, V. Stavila, and M. D. Allendorf. "An Analytical Bond Order Potential for Mg-H Systems." *ChemPhysChem* 20 (2019): 1404.
<https://doi.org/10.1002/cphc.201800991>.

2018

Allendorf, M. D., Z. Hulvey, T. Gennett, A. Alauddin, S. Autrey, J. Camp, and E. Cho, et al. "An Assessment of Strategies for the Development of Solid-State Adsorbents for Vehicular Hydrogen Storage." *Energy & Environmental Science* 11, no. 10 (2018): 2784–2812. <https://doi.org/10.1039/c8ee01085d>.

Camp, J., V. Stavila, M. D. Allendorf, D. Prendergast, and M. Haranczyk. "Critical Factors in Computational Characterization of Hydrogen Storage in Metal-Organic Frameworks." *Journal of Physical Chemistry C* 122, no. 33 (2018): 18957–18967.

Carr, C. L., W. Jayawardana, H. Y. Zou, J. L. White, F. El Gabaly, M. S. Conradi, V. Stavila, M. D. Allendorf, and E. H. Majzoub. "Anomalous H₂ Desorption Rate of NaalH₄ Confined in Nitrogen-Doped Nanoporous Carbon Frameworks." *Chemistry of Materials* 30, no. 9 (2018): 2930–2938.

Dimitrievska, M., J. N. Chotard, R. Janot, A. Faraone, W. S. Tang, A. V. Skripov, and T. J. Udovic. "Tracking the Progression of Anion Reorientational Behavior between Alpha-Phase and Beta-Phase Alkali-Metal Silanides, Msih₃, by Quasielastic Neutron Scattering." *Journal of Physical Chemistry C* 122, no. 42 (2018): 23985–23997.

Dimitrievska, M., P. Shea, K. E. Kweon, M. Bercx, J. B. Varley, W. S. Tang, A. V. Skripov, et al. "Carbon Incorporation and Anion Dynamics as Synergistic Drivers for Ultrafast Diffusion in Superionic Licb11h12 and Nacb11h12." *Advanced Energy Materials* 8, no. 15 (2018).

Dimitrievska, M., V. Stavila, A. V. Soloninin, R. V. Skoryunov, O. A. Babanova, H. Wu, W. Zhou, et al. "Nature of Decahydro-Closo-Decaborate Anion Reorientations in an Ordered Alkali-Metal Salt: Rb₂b₁₀h₁₀." *Journal of Physical Chemistry C* 122, no. 27 (2018): 15198–15207.

Jensen, S. R. H., M. Paskevicius, B. R. S. Hansen, A. S. Jakobsen, K. T. Moller, J. L. White, M. D. Allendorf, et al. "Hydrogenation Properties of Lithium and Sodium Hydride - Closo-Borate, [B₁₀h₁₀](²⁻) and [B₁₂h₁₂](²⁻), Composites." *Physical Chemistry Chemical Physics* 20, no. 23 (2018): 16266–16275.

Kang, S., L. E. Klebanoff, A. A. Baker, D. F. Cowgill, V. Stavila, J. R. I. Lee, M. H. Nielsen, et al. "Assessing the Reactivity of Ticl₃ and Tif₃ with Hydrogen." *International Journal of Hydrogen Energy* 43, no. 31 (2018): 14507–14519.

Kapelewski, M. T., T. Runcevski, J. D. Tarver, H. Z. H. Jiang, K. E. Hurst, P. A. Parilla, A. Ayala, et al. "Record High Hydrogen Storage Capacity in the Metal-Organic Framework Ni-2(M-Dobdc) at near-Ambient Temperatures." *Chemistry of Materials* 30, no. 22 (2018): 8179–8189.

Melaet, G., V. Stavila, L. Klebanoff, and G. A. Somorjai. "The Effect of Aluminum and Platinum Additives on Hydrogen Adsorption on Mesoporous Silicates." *Physical Chemistry Chemical Physics* 20, no. 17 (2018): 12075–12083.

Muller, K., K. Brooks, and T. Autrey. "Releasing Hydrogen at High Pressures from Liquid Carriers: Aspects for the H₂ Delivery to Fueling Stations." *Energy & Fuels* 32, no. 9 (2018): 10008–10015.
<https://doi.org/10.1021/acs.energyfuels.8b01724>.

Schneemann, A., J. L. White, S. Kang, S. Jeong, L. W. F. Wan, E. S. Cho, T. W. Heo, *et al.* “Nanostructured Metal Hydrides for Hydrogen Storage.” *Chemical Reviews* 118, no. 22 (2018): 10775–10839.

Skripov, A. V., R. V. Skoryunov, A. V. Soloninin, O. A. Babanova, V. Stavila, and T. J. Udovic. “Nuclear Magnetic Resonance Study of Anion and Cation Reorientational Dynamics in (Nh₄)₂B₁₂H₁₂.” *Journal of Physical Chemistry C* 122, no. 6 (2018): 3256–3262.

Zhou, X. W., T. W. Heo, B. C. Wood, V. Stavila, S. Kang, and M. D. Allendorf. “Molecular Dynamics Studies of Fundamental Bulk Properties of Palladium Hydrides for Hydrogen Storage.” *Journal of Applied Physics* 123, no. 22 (2018).

Zhou, X. W., T. W. Heo, B. C. Wood, V. Stavila, S. Kang, and M. D. Allendorf. “Temperature- and Concentration-Dependent Hydrogen Diffusivity in Palladium from Statistically-Averaged Molecular Dynamics Simulations.” *Scripta Materialia* 149 (2018): 103–107.

<https://doi.org/10.1016/j.scriptamat.2018.02.010>.

Zhu, Q. L., F. Z. Song, Q. J. Wang, N. Tsumori, Y. Himeda, T. Autrey, and Q. Xu. “A Solvent-Switched in Situ Confinement Approach for Immobilizing Highly-Active Ultrafine Palladium Nanoparticles: Boosting Catalytic Hydrogen Evolution.” *Journal of Materials Chemistry A* 6, no. 14 (2018): 5544–5549.

2017

Cho, E. S., F. Qiu, and J. J. Urban. “Tailoring Polymer Conformation for Nanocrystal Growth: The Role of Chain Length and Solvent.” *Small* 13, no. 3 (2017). <https://doi.org/10.1002/sml.201602572>.

Cho, E. S., A. M. Ruminski, Y. S. Liu, P. T. Shea, S. Y. Kang, E. W. Zaia, J. Y. Park, *et al.* “Hierarchically Controlled inside-out Doping of Mg Nanocomposites for Moderate Temperature Hydrogen Storage.” *Advanced Functional Materials* 27, no. 47 (2017).

DeSantis, D., J. A. Mason, B. D. James, C. Houchins, J. R. Long, and M. Veenstra. “Techno-Economic Analysis of Metal-Organic Frameworks for Hydrogen and Natural Gas Storage.” *Energy & Fuels* 31, no. 2 (2017): 2024–2032.

Kang, S., T. Ogitsu, S. A. Bonev, T. W. Heo, M. D. Allendorf, and B. C. Wood. “Understanding Charge Transfer at Mg/MgH₂ Interfaces for Hydrogen Storage.” *Solid-Gas Electrochemical Interfaces 2 (Sgei 2)* 77, no. 10 (2017): 81–90. <https://doi.org/10.1149/07710.0081ecst>.

Li, Z. P., X. C. Yang, N. Tsumori, Z. Liu, Y. Himeda, T. Autrey, and Q. Xu. “Tandem Nitrogen Functionalization of Porous Carbon: Toward Immobilizing Highly Active Palladium Nanoclusters for Dehydrogenation of Formic Acid.” *ACS Catalysis* 7, no. 4 (2017): 2720–2724.

Muller, K., K. Brooks, and T. Autrey. “Hydrogen Storage in Formic Acid: A Comparison of Process Options.” *Energy & Fuels* 31, no. 11 (2017): 12603–12611.

Ray, K. G., L. E. Klebanoff, J. R. I. Lee, V. Stavila, T. W. Heo, P. Shea, A. A. Baker, *et al.* “Elucidating the Mechanism of MgH₂ Initial Hydrogenation Via a Combined Experimental-Theoretical Study.” *Physical Chemistry Chemical Physics* 19, no. 34 (2017): 22646–22658. <https://doi.org/10.1039/c7cp03709k>.

Soloninin, A. V., M. Dimitrievska, R. V. Skoryunov, O. A. Babanova, A. V. Skripov, W. S. Tang, V. Stavila, S. Orimo, and T. J. Udovic. “Comparison of Anion Reorientational Dynamics in M_{cb}(9)Hi(10) and M_{2b}10h10

(M = Li, Na) Via Nuclear Magnetic Resonance and Quasielastic Neutron Scattering Studies." *Journal of Physical Chemistry C* 121, no. 2 (2017): 1000–1012.

Tang, W. S., M. Dimitrievska, V. Stavila, W. Zhou, H. Wu, A. A. Talin, and T. J. Udovic. "Order-Disorder Transitions and Superionic Conductivity in the Sodium Nido-Undeca(Carba)Borates." *Chemistry of Materials* 29, no. 24 (2017): 10496–10509. <https://doi.org/10.1021/acs.chemmater.7b04332>.

Tsivion, E., and M. Head-Gordon. "Methane Storage: Molecular Mechanisms Underlying Room Temperature Adsorption in Zn₄o(Bdc)(3) (Mof-5)." *Journal of Physical Chemistry C* 121, no. 22 (2017): 12091–12100.

Tsivion, E., S. P. Veccham, and M. Head-Gordon. "High-Temperature Hydrogen Storage of Multiple Molecules: Theoretical Insights from Metalated Catechols." *Chemphyschem* 18, no. 2 (2017): 184–188.

Wan, L. W. F., Y. S. Liu, E. S. Cho, J. D. Forster, S. Jeong, H. T. Wang, J. J. Urban, J. H. Guo, and D. Prendergast. "Atomically Thin Interfacial Suboxide Key to Hydrogen Storage Performance Enhancements of Magnesium Nanoparticles Encapsulated in Reduced Graphene Oxide." *Nano Letters* 17, no. 9 (2017): 5540–5545. <https://doi.org/10.1021/acs.nanolett.7b02280>.

Wood, B. C., V. Stavila, N. Poonyayant, T. W. Heo, K. G. Ray, L. E. Klebanoff, T. J. Udovic, *et al.* "Nanointerface-Driven Reversible Hydrogen Storage in the Nanoconfined Li-N-H System." *Advanced Materials Interfaces* 4, no. 3 (2017).

X. W. Zhou, T. W. Heo, B. C. Wood, V. Stavila, S. Kang, and M. D. Allendorf "Finite-Temperature Behavior of Pd₁₀ Elastic Constants Computed by Direct Molecular Dynamics." *MRS Advances* 2, no. 55 (2017): 3341–3346. <https://doi.org/10.1557/adv.201.387>.

2016

Brooks, K. P., M. E. Bowden, A. J. Karkamkar, A. Y. Houghton, and S. T. Autrey. "Coupling of Exothermic and Endothermic Hydrogen Storage Materials." *Journal of Power Sources* 324 (2016): 170–178.

Broom, D. P., C. J. Webb, K. E. Hurst, P. A. Parilla, T. Gennett, C. M. Brown, R. Zacharia, *et al.* "Outlook and Challenges for Hydrogen Storage in Nanoporous Materials." *Applied Physics a-Materials Science & Processing* 122, no. 3 (2016).

Callini, E., Z. O. K. Atakli, B. C. Hauback, S. Orimo, C. Jensen, M. Dornheim, D. Grant, *et al.* "Complex and Liquid Hydrides for Energy Storage." *Applied Physics a-Materials Science & Processing* 122, no. 4 (2016).

Cho, E. S., A. M. Ruminski, S. Aloni, Y. S. Liu, J. H. Guo, and J. J. Urban. "Graphene Oxide/Metal Nanocrystal Multilaminates as the Atomic Limit for Safe and Selective Hydrogen Storage (Vol 7, 10804, 2016)." *Nature Communications* 7 (2016).

Gygi, D., E. D. Bloch, J. A. Mason, M. R. Hudson, M. I. Gonzalez, R. L. Siegelman, T. A. Darwish, *et al.* "Hydrogen Storage in the Expanded Pore Metal-Organic Frameworks M-2(Dobpdc) (M = Mg, Mn, Fe, Co, Ni, Zn)." *Chemistry of Materials* 28, no. 4 (2016): 1128–1138.

Hurst, K. E., P. A. Parilla, K. J. O'Neill, and T. Gennett. "An International Multi-Laboratory Investigation of Carbon-Based Hydrogen Sorbent Materials." *Applied Physics a-Materials Science & Processing* 122, no. 1 (2016).

- Levine, D. J., T. Runcevski, M. T. Kapelewski, B. K. Keitz, J. Oktawiec, D. A. Reed, J. A. Mason, *et al.* "Olsalaiine-Based Metal-Organic Frameworks as Biocompatible Platforms for H₂ Adsorption and Drug Delivery." *Journal of the American Chemical Society* 138, no. 32 (2016): 10143–10150.
- Parilla, P. A., K. Gross, K. Hurst, and T. Gennett. "Recommended Volumetric Capacity Definitions and Protocols for Accurate, Standardized and Unambiguous Metrics for Hydrogen Storage Materials." *Applied Physics a-Materials Science & Processing* 122, no. 3 (2016).
- Runcevski, T., M. T. Kapelewski, R. M. Torres-Gavosto, J. D. Tarver, C. M. Brown, and J. R. Long. "Adsorption of Two Gas Molecules at a Single Metal Site in a Metal-Organic Framework." *Chemical Communications* 52, no. 53 (2016): 8251–8254.
- Tang, W. S., M. Dimitrievska, J. N. Chotard, W. Zhou, R. Janot, A. V. Skripov, and T. J. Udovic. "Structural and Dynamical Trends in Alkali-Metal Silanides Characterized by Neutron-Scattering Methods." *Journal of Physical Chemistry C* 120, no. 38 (2016): 21218–21227.
- Tang, W. S., K. Yoshida, A. V. Soloninin, R. V. Skoryunov, O. A. Babanova, A. V. Skripov, M. Dimitrievska, *et al.* "Stabilizing Superionic-Conducting Structures Via Mixed-Anion Solid Solutions of Monocarba-Closo-Borate Salts." *ACS Energy Letters* 1, no. 4 (2016): 659–664.
- Whittemore, S. M., M. Bowden, A. Karkamkar, K. Parab, D. Neiner, T. Autrey, J. S. A. Ishibashi, *et al.* "Blending Materials Composed of Boron, Nitrogen and Carbon to Transform Approaches to Liquid Hydrogen Stores." *Dalton Transactions* 45, no. 14 (2016): 6196–6203.
- Wood, K. N., S. T. Christensen, D. Nordlund, A. A. Dameron, C. Ngo, H. Dinh, T. Gennett, R. O'Hayre, and S. Pylypenko. "Spectroscopic Investigation of Nitrogen-Functionalized Carbon Materials." *Surface and Interface Analysis* 48, no. 5 (2016): 283–292.
- Wu, H., W. S. Tang, W. Zhou, J. D. Tarver, V. Stavila, C. M. Brown, and T. J. Udovic. "The Low-Temperature Structural Behavior of Sodium 1-Carba-Closo-Decaborate: Nacb9h10." *Journal of Solid State Chemistry* 243 (2016): 162–167.
- Wu, H., X. Q. Zhou, E. E. Rodriguez, W. Zhou, T. J. Udovic, T. Yildirim, and J. J. Rush. "A New Family of Metal Borohydride Guanidinate Complexes: Synthesis, Structures and Hydrogen-Storage Properties." *Journal of Solid State Chemistry* 242 (2016): 186–192.
- Zhou, X. W., F. El Gabaly, V. Stavila, and M. D. Allendorf. "Molecular Dynamics Simulations of Hydrogen Diffusion in Aluminum." *Journal of Physical Chemistry C* 120, no. 14 (2016): 7500–7509.