Vitalie Stavila

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| **EDUCATION** |

* **Ph.D. / Inorganic Chemistry**

State University of Moldova, Chisinau, Moldova, 2002

Thesis title: “Synthesis of new bismuth-transition metal heterometallic complexes as molecular precursors for mixed oxide systems”

* **B.S. / Chemistry**

State University of Moldova, Chisinau, Moldova, 1996

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| **PROFESSIONAL EXPERIENCE** |

* **2008 – present**

***Research Scientist***

Principal investigator on an U.S. Department of Energy sponsored project devoted to synthesis of materials for reversible hydrogen storage

Development of multifunctional materials for energy applications, including electrolytes for solid-state batteries, membranes for fuel cells and catalysis for biomass valorization

Fabrication of nanoparticles, thin films, and coatings as active materials in functional devices

Management of the Sandia-California X-ray diffraction facility

* **2005 – 2007**

***Postdoctoral Research Associate***

Department of Chemistry, Rice University, Houston, TX

Research on organometallic and inorganic complexes as precursors for nanostructured alloys, oxide and chalcogenide nanostructured materials

* **2004 – 2005**

***Postdoctoral Fellow***

Ecole Normale Supérieure de Lyon, France

Design and synthesis of enzyme-responsive iron complexes as Magnetic Resonance Imaging (MRI) contrast agents

* **2002 – 2004**

***Lecturer***

Department of Chemistry, State University of Moldova, Chisinau, Moldova

* **1996 – 2002**

***Graduate Studies,*** Advisor: *Prof. Aurelian Gulea*

State University of Moldova, Chisinau, Moldova

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| **TECHNICAL EXPERIENCE** |

* Design, synthesis and characterization of solid-state hydrogen storage materials; mechanistic studies of the hydrogen release and absorption in bulk and nanoscale metal hydride materials and the effect of additives and catalysts on their cycling characteristics.
* Main group and transition metal inorganic and organometallic chemistry including synthesis, purification and characterization of air-sensitive compounds with emphasis on the use of Schlenk-line techniques and inert atmosphere dry-boxes.
* Synthesis and characterization of bulk and nano-materials, including hydrides, oxides and chalcogenides with controlled chemical compositions and morphologies using hydrothermal, solid-state, solution, hydrothermal and solvothermal techniques.
* Structural characterization of molecules and materials by X-ray and neutron diffraction techniques; extensive experience with powder and single-crystal structure refinement.
* Gibbs Free Energy Minimization calculations using *FactSage* to elucidate reaction kinetics as well as thermodynamics of bulk and nanoscale complex metal hydrides.
* Instrumental analysis: hydrogen desorption/absorption kinetics and pressure-composition-isotherms measurements using Sievert’s and PCT instruments, 1H, 13C, 11B, 27Al NMR, TGA/TDA/MS, DSC, FTIR, UV-VIS, LC-MS, GS-MS, HPLC, UV-VIS, TEM, SEM, EDS, RGA.
* Computer skills: *Software* – ChemDraw, EndNote, Photoshop, Corel; *Structural refinement* – SHELXTL, PLATON, MERCURY, JADE, NANO-Solver; *Databases* – CSD, ICSD, SciFinder.

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| **HONORS AND AWARDS** |

Sandia Employee Recognition Award, December 2015; November 2018

U.S. DOE Hydrogen Program “Special Recognition Award” for the MHCoE team, June 2010

Welch Fellowship, Department of Chemistry, Rice University, May 2006-August 2007

Civilian Research and Development Foundation Research Award, 2006

NSF-NATO Postdoctoral Fellowship Award, May 2005 – May 2006

Young Scientist of the Year Award, Moldova, Chisinau, April 2004

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| **PROFESSIONAL MEMBERSHIP** |

American Chemical Society, Materials Research Society, American Association for the Advancement of Science, International Association for Hydrogen Energy

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| **SYNERGISTIC ACTIVITIES** |

Proposal Reviewer: *DOE EERE, ARPA-E, NSF, CRDF, INTAS, SCOPES*

Editorial Board Member: *Frontiers in Energy Storage, Materials*

Journal Reviewer: *Science, Nature*, *Journal of the American Chemical Society*, *Angewandte Chemie*, *Chemical Communications*, *Chemistry of Materials, Journal of Materials Chemistry, Inorganic Chemistry, Journal of Physical Chemistry, Energy & Environmental Science, CrystEngComm, European Journal of Inorganic Chemistry, Inorganic Chemistry Communications, Journal of Cluster Science, , International Journal of Hydrogen Energy, Microporous & Mesoporous Materials, Crystal Growth & Design*

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| **PUBLICATIONS** |

(Co)-authored >160 research publications and review articles (h-index = 57; about 12,500 total citations), 2 book chapters, 15 US and international patents, and >90 conference contributions.

**Publication list (as of May 2022)**

**Peer-Reviewed Journal Articles:**

1. Luning Chen, Pragya Verma, Kaipeng, Hou, Zhiyuan Qi, Shuchen Zhang, Yi-Sheng Liu, Jinghua Guo, Vitalie Stavila, Mark D. Allendorf, David Prendergast, Gabor A. Somorjai, Ji Su, “Reversible dehydrogenation and rehydrogenation of cyclohexane and methylcyclohexane by single-site platinum catalyst”, *Nature Communications*, **2022**, *13*, 1092. DOI:10.1038/s41467-022-28607-y.
2. Keith G. Ray, Leonard E. Klebanoff, Vitalie Stavila, ShinYoung Kang, Liwen F. Wan, Sichi Li, Tae Wook Heo, Mark D. Allendorf, Jonathan R. I. Lee, Alexander A. Baker, and Brandon C. Wood, “Understanding Hydrogenation Chemistry at MgB2 Reactive Edges from Ab Initio Molecular Dynamics”, *ACS Applied Materials & Interfaces*, **2022**, 14, 20430-20442. DOI: 10.1021/acsami.1c23524.
3. Matthew Green, Katty Kaydanik, Miguel Orozco, Lauren Hanna, Maxwell Marple, Kimberly Fessler, Willis Jones, Vitalie Stavila, Patrick A. Ward, Joseph A. Teprovich, “*Closo*-Borate Gel Polymer Electrolyte with Remarkable Electrochemical Stability and a Wide Operating Temperature Window”, *Advanced Science*, **2022**, 2106032. DOI:10.1002/advs.202106032
4. N. A. Strange, N. Leick, S. Shulda, A. Schneemann, V. Stavila, A. S. Lipton, M. F. Toney, T. Gennett, S. T. Christensen, “Reactive Vapor-Phase Additives toward Destabilizing γ-Mg(BH4)2 for Improved Hydrogen Release” *ACS Applied Energy Materials*, **2022***, 5,* 1690–1700*.* DOI: 10.1021/acsaem.1c03128
5. C. Dun, S. Jeong, Y.-S. Liu, N. Leick, T. M. Mattox, J. Guo, J.-W. Lee, T. Gennett, V. Stavila, J. J. Urban, “Hydrogen storage performance of preferentially oriented Mg/rGO hybrids” *Chemistry of Materials*, **2022***, 34,* 2963-2971*.* DOI: 10.1021/acs.chemmater.1c03714
6. J. A. Pérez-Pimienta, G. Papa, J. Sun, V. Stavila, A. Sanchez, J. M. Gladden, B. A. Simmons “One-pot ethanol production under optimized pretreatment conditions using agave bagasse at high solids loading with low-cost biocompatible protic ionic liquid” *Green Chemistry* **2022***, 24*, 207-217*.* DOI:10.1039/D1GC03774A
7. J. L. Snider, Y.-S. Liu, A. M. Sawvel, L. F. Wan, V. Stavila, T.M. Mattox, P. Wijeratne, M.D. Allendorf, B.C. Wood, L.E. Klebanoff, “The influence of LiH and TiH2 on hydrogen storage in MgB2 I: Promotion of bulk hydrogenation at reduced temperature” *Int. J. Hydrogen Energy*, **2022***, 47,* 387-402*.* DOI:10.1016/j.ijhydene.2021.09.169
8. J. L. Snider, T. M. Mattox, Y.-S. Liu, L. F. Wan, P. Wijeratne, M. D. Allendorf, V. Stavila, B. C. Wood, L. E. Klebanoff, “The influence of LiH and TiH2 on hydrogen storage in MgB2 II. XPS study of surface and near-surface phenomena” *Int. J. Hydrogen Energy*, **2022***, 47*, 403-419*.* DOI:10.1016/j.ijhydene.2021.09.163
9. V. Stavila, S. C. Li, C. Dun, M. A. T. Marple, H. E. Mason, J. L. Snider, J. E. Reynolds, F. El Gabaly, J. D. Sugar, C. D. Spataru, X. W. Zhou, B. Dizdar, E. H. Majzoub, R. Chatterjee, J. Yano, H. Schlomberg, B. V. Lotsch, J. J. Urban, B. C. Wood, M. D. Allendorf “Defying Thermodynamics: Stabilization of Alane Within Covalent Triazine Frameworks for Reversible Hydrogen Storage” *Angew. Chem. Int. Ed.* (**2021**) DOI: 10.1002/anie.202107507. Hot Paper, journal inside cover*.*
10. Y. Cho, S. Li, J. L. Snider, M. A. T. Marple, N. A. Strange, J. D. Sugar, F. El Gabaly, A. Schneemann, S. Kang, M. Kang, H. Park, J. Park, L. F. Wan, H. E. Mason, M. D. Allendorf, B. C. Wood, E. S. Cho, V. Stavila “Reversing the Irreversible: Thermodynamic Stabilization of Lithium Aluminum Hydride Nanoconfined Within a Nitrogen-Doped Carbon Host” *ACS Nano* **2021***, 15,* 10163-10174*.* DOI:10.1021/acsnano.1c02079
11. M. Witman, G. Ek, S. Ling, J. M. Chames, S. Agarwal, J. Wong, M. D. Allendorf, M. Sahlberg, V. Stavila *Chem. Mater.* “Data-driven discovery and synthesis of high entropy alloy hydrides with targeted thermodynamic stability” *Chem. Mater.* **2021**, *33*, 4067 DOI: [10.1021/acs.chemmater.1c00647](https://doi.org/10.1021/acs.chemmater.1c00647) Journal cover*.*
12. J. L. Snider, J. Su, P. Verma, F. El Gabaly, J. D. Sugar, L. N. Chen, J. M. Chames, A. A. Talin, C. C. Dun, J. J. Urban, V. Stavila, D. Prendergast, G. A. Somorjai, M. D. Allendorf “Stabilized open metal sites in bimetallic metal-organic framework catalysts for hydrogen production from alcohols” *J. Mater. Chem. A* **2021,** *9*, 10869.
13. M. D. Allendorf, V. Stavila, M. Witman, C. K. Brozek, C. H. Hendon “What lies beneath a Metal-Organic Framework crystal structure? New design principles from unexpected behaviors” *J. Amer. Chem. Soc.* **2021**, *143*, 6705.
14. S. Yoon, A. A. Talin, V. Stavila, A. M. Mroz, T. D. Bennett, Y. He, D. A. Keen, C. H. Hendon, M. D. Allendorf, M. C. So “From n- to p-Type Material: Effect of Metal Ion on Charge Transport in Metal–Organic Materials” *ACS Appl. Mater. Interfaces* **2021**, [doi.org/10.1021/acsami.1c09130](https://doi.org/10.1021/acsami.1c09130).
15. S. Li, H. Gunda, K. G. Ray, C.-S. Wong, P. Xiao, R. W. Friddle, Y. -S. Liu, S. Kang, C. Dun, J. D. Sugar, R. D. Kolasinski, L. F. Wan, A. A. Baker, J. R. I. Lee, J. J. Urban,K. Jasuja, M. D. Allendorf, V. Stavila, B. C. Wood “Spontaneous dynamical disordering of borophenes in MgB2 and related metal borides” *Nat. Commun.* **12,** 6268 (**2021**). doi.org/10.1038/s41467-021-26512-4.
16. Dun, C.; Jeong, S.; Liu, Y.-S.; Leick, N.; Mattox, T.M.; Guo, J.H.; Lee, J.W.; Gennett, T. Stavila, V.; Urban, J.J. Additive Destabilization of Porous Magnesium Borohydride Framework with Core-Shell Structure, *Small*, *2021*, *17*, 2101989.
17. Andersson, M.S.; Stavila, V.; Skripov, A.V.; Dimitrievska, M. Psurek, M.T.; Leao, J.B.; Babanova, O.A.; Skoryunov, R.V.; Soloninin, A.V.; Karlsson, M.; Udovic, T.J. (Udovic, Terrence J.). "Promoting Persistent Superionic Conductivity in Sodium Monocarba-closo-dodecaborate NaCB11H12 via Confinement within Nanoporous Silica" *Journal of Physical Chemistry* *C,* **2021**,*125*, 16689-16699.
18. Gunda, H.; Klebanoff, L.E.; Sharma, P.A.; Varma, A.K.; Dolia, V.; Jasuja, K.; Stavila, V. “Progress, Challenges, and Opportunities in the Synthesis, Characterization, and Application of Metal-Boride-Derived Two-Dimensional Nanostructures” *ACS Materials Letters*, **2021**, *3*, 535-556.
19. M. Witman, S. L. Ling, D. M. Grant, G. S. Walker, S. Agarwal, V. Stavila, M. D. Allendorf “Extracting an Empirical Intermetallic Hydride Design Principle from Limited Data via Interpretable Machine Learning” *J. Phys. Chem. Lett.* **2020**, *11*, 40.
20. 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” *Adv. Mater. Interfaces* **2020**, *7*, 1901905. Journal cover.
21. J. L. White N.A. Strange, J. D. Sugar, J. L. Snider, A. Schneemann, A. S. Lipton, M. F. Tony, M. D. Allendorf, V. Stavila “Melting of Magnesium Borohydride under High Hydrogen Pressure: Thermodynamic Stability and Effects of Nanoconfinement” *Chem. Mater.*, **2020**, *32*, 5604.
22. 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, J. Jorgensen, T. R. Jensen, B. C. Wood, M. D. Allendorf, V. Stavila “Nanoconfinement of Molecular Magnesium Borohydride Captured in a Bipyridine-Functionalized Metal-Organic Framework” *ACS Nano*, **2020**, *14,* 10294.
23. M. D. Allendorf, R. Dong, X. Feng, S. Kaskel, D. Matoga, V. Stavila “Electronic Devices Using Open Framework Materials” *Chem. Rev.* **2020**, 120, 16, 8581.
24. C. D. Spataru, T. W. Heo, B. C. Wood, V. Stavila, S. Kang, M. D. Allendorf, X. W. Zhou “Statistically Averaged Molecular Dynamics Simulations of Hydrogen Diffusion in Magnesium and Magnesium Hydrides” *Phys. Rev. Mater.* **2020**, *4*, 105401.
25. M. Witman, S. Ling, V. Stavila, P. Wijeratne, H. Furukawa, M. D. Allendorf “Design principles for the ultimate gas deliverable capacity material: nonporous to porous deformations without volume change” *Molec. Syst. Design. Eng.* **2020**, *5*, 1491-1498.
26. Vitalie Stavila, Michael E. Foster, Jonathan W. Brown, Ryan W. Davis, Jane Edgington, Annabelle I. Benin, Ryan A. Zarkesh, Ramakrishnan Parthasarathi, David W. Hoyt, Eric D. Walter, Amity Andersen, Nancy M. Washton, Andrew S. Lipton, Mark D. Allendorf, *Chemical Science*, **2019**, DOI:10.1039/C9SC01018A; “IRMOF-74(n)–Mg: a novel catalyst series for hydrogen activation and hydrogenolysis of C–O bonds”
27. Timothy C. Wang, Patrick F. Doty, Annabelle Benin, Joshua D. Sugar, Vitalie Stavila, Mark D. Allendorf,

*Chemical Communications*, **2019**, *55*, 4647-4650.

“Get the light out: nanoscaling MOFs for luminescence sensing and optical applications”

1. Yi‐Sheng Liu, Sohee Jeong, James L. White, Xuefei Feng, Eun Seon Cho, Vitalie Stavila, Mark D. Allendorf, Jeffrey J. Urban, Jinghua Guo. *ChemPhysChem,* **2019**, *20,* 1261-1271*.*

”In‐Situ/Operando X‐ray Characterization of Metal Hydrides”

1. Timothy C. Wang, James L. White, Binglin Bie, Hexiang Deng, Jane Edgington, Joshua D. Sugar, Vitalie Stavila, Mark D. Allendorf, *ChemPhysChem,* **2019***, 20,* 1305-1310**.**

“Design Rules for Metal-Organic Framework Stability in High-Pressure Hydrogen Environments”

1. Cody Sugai, Stephen Kim, Godwin Severa, James L. White, Noemi Leick, Madison B. Martinez, Thomas Gennett, Vitalie Stavila, Craig Jensen, *ChemPhysChem,* **2019**, *20*, 1301-1304.

”Kinetic “Enhancement of Direct Hydrogenation of MgB2 to Mg(BH4)2 upon Mechanical Milling with THF, MgH2, and/or Mg”

1. Xiaowang Zhou, Shinyoung Kang, Tae-Wook Heo, Brandon Wood, Vitalie Stavila, Mark. D. Allendorf, *ChemPhysChem,* **2019**, *20*, 1404-1311.

“An Analytical Bond Order Potential for Mg-H Systems”

1. White, J.L.; Rowberg, A.J.E.; Wan, L.W.F.; Kang, S.; Ogitsu, T.; Kolasinski, R.D.; Whaley, J.A.; Baker, A.A.; Lee, J.R.I.; Liu, Y.-S.; Trotochaud, L.; Guo, J.G.; Stavila, V.; Prendergast, D.; Bluhm, H.; Allendorf, M.D.; Wood, B.C.; El Gabaly, F. *ACS Applied Materials and Interfaces,* **2019,** *11*, 4930-4941.

”Identifying the Role of Dynamic Surface Hydroxides in the Dehydrogenation of Ti-Doped NaAlH4”

1. Fang Liu, Pamela Lane, John C. Hewson, Vitalie Stavila, Mary B.Tran-Gyamfi, Michele Hamel, Todd W.Lane, Ryan W.Davis, *Bioresource Technology*, **2019**, *283*, 350-357.

“Development of a closed-loop process for fusel alcohol production and nutrient recycling from microalgae biomass”

1. José A. Pérez Pimienta, Gabriella Papa, Alberto Rodriguez, Carolina A. Barcelos, Ling Liang, Vitalie Stavila, Arturo Sanchez, John M. Gladden, Blake A. Simmons, *Green Chemistry*, **2019**, *21*, 3152-3164.

“Pilot-scale hydrothermal pretreatment and optimized saccharification enables bisabolene production from multiple feedstocks”

1. Schneemann, A.; White, J. L.; Kang, SY.; Jeong, S.; Wan, L. F.; Cho, E. S.; Heo, T. W.; Prendergast, D.; Urban, J. J.; Wood, B. C.; Allendorf, M. D.; Stavila, V. *Chemical Reviews,* **2018,** *118*, 10775-10839.

”Nanostructured Metal Hydrides for Hydrogen Storage”

1. Allendorf, M.D.; Hulvey, Z.; Gennett, T.; Ahmed, A.; Autrey, T.; Camp, J.; Cho, E. S.; Furukawa, H.; Haranczyk, M.; Head-Gordon, M.; Jeong, S.; Karkamkar, A.; Liu, D.-J.; Long, J. R.; Meihaus, K. R.; Nayyar, I. H.; Nazarov, R.; Siegel, D. J.; Stavila, V.; Urban, J. J Veccham S. P.; Wood, B.C., *Energy and Environmental Science,* **2018,** *11*, 2784-2812.

”An Assessment of Strategies for the Development of Solid-State Adsorbents for Vehicular Hydrogen Storage”

1. Thurmer, K.; Schneider, C.; Stavila, V.; Friddle, R.W.; Leonard, F.; Fischer, R.A.; Allendorf, M.D.; Talin, A.A. *ACS Applied Materials and Interfaces,* **2018,** *10*, 39400-39410.

”Surface Morphology and Electrical Properties of Cu3BTC2 Thin Films Before and After Reaction with TCNQ”

1. Vajo, J. J.; Tan, H.; Ahn, C. C.; Addison, D.; Hwang, S.-J.; White, J. L.; Wang, T. C.; Stavila, V.; Graetz, J. *Journal of Physical Chemistry* *C,* **2018,** *122*, 26845-26850.

”Electrolyte-Assisted Hydrogen Storage Reactions”

1. Dimitrievska, M.; Shea, P.; Kweon, K. E.; Bercx, M.; Varley, J. B.; Tang, W. S.; Skripov, A. V.; Stavila, V.; Udovic, T. J.; Wood, B. C. *Advanced Energy Materials* **2018,** *8*, 1703422.

”Carbon Incorporation and Anion Dynamics as Synergistic Drivers for Ultrafast Diffusion in Superionic LiCB11H12 and NaCB11H12”

1. Carr, C. L.; Jayawardana, W.; Zou, H. Y.; White, J. L.; El Gabaly, F.; Conradi, M. S.; Stavila, V.; Allendorf, M. D.; Majzoub, E. H. *Chemistry of Materials* **2018,** *30*, 2930-2938.

”Anomalous H2 Desorption Rate of NaAlH4 Confined in Nitrogen-Doped Nanoporous Carbon Frameworks”

1. Camp, J.; Stavila, V.; Allendorf, M. D.; Prendergast, D.; Haranczyk. *Journal of Physical Chemistry C* **2018,** *122*, 18957-18967.

”Critical Factors in Computational Characterization of Hydrogen Storage in Metal-Organic Frameworks”

1. Dimitrievska, M.; Stavila, V.; Soloninin, A. V.; Skoryunov, R. V.; Babanova, O. A.; Wu, H.; Zhou, W.; Tang, W. S.; Faraone, A.; Tarver, J. D.; Trump, B. A.; Skripov, A. V.; Udovic, T. J. *Journal of Physical Chemistry C* **2018,** *122*, 15198-15207.

”Nature of Decahydro-closo-decaborate Anion Reorientations in an Ordered Alkali-Metal Salt: Rb2B10H10”

1. Jensen, S. R. H.; Paskevicius, M.; Hansen, B. R. S.; Jakobsen, A. S.; Moller, K. T.; White, J. L.; Allendorf, M. D.; Stavila, V.; Skibsted, J.; Jensen, T. R. *Physical Chemistry Chemical Physics* **2018,** *20*, 16266-16275.

”Hydrogenation properties of lithium and sodium hydride - *closo*-borate, B10H10(2-) and B12H12(2-), composites.”

1. Melaet, G.; Stavila, V.; Klebanoff, L.; Somorjai, G. A. *Physical Chemistry Chemical Physics* **2018,** *20*, 12075-12083.

”The effect of aluminum and platinum additives on hydrogen adsorption on mesoporous silicates”

1. Kang, S.; Klebanoff, L. E.; Baker, A. A.; Cowgill, D. F.; Stavila, V.; Lee, J. R. I.; Nielsen, M. H.; Ray, K. G.; Liu, Y. S.; Wood, B. C. *International Journal of Hydrogen Energy* **2018,** *122*, 3256-3262.

”Assessing the reactivity of TiCl3 and TiF3 with hydrogen”

1. Zhou, X. W.; Heo, T. W.; Wood, B. C.; Stavila, V.; Kang, S.; Allendorf, M. D., T. J. *Scripta Materialia* **2018,** *149*, 103-107.

”Temperature- and concentration-dependent hydrogen diffusivity in palladium from statistically-averaged molecular dynamics simulations”

1. Zhou, X. W.; Heo, T. W.; Wood, B. C.; Stavila, V.; Kang, S.; Allendorf, M. D. *Journal of Applied Physics* **2018,** *123*, 225105.

”Molecular dynamics studies of fundamental bulk properties of palladium hydrides for hydrogen storage”

1. Ullman, A. M.; Jones, C. G.; Doty, F. P.; Stavila, V.; Talin, A. A.; Allendorf, M. D. *ACS Applied Materials & Interfaces* **2018,** *10*, 24201-24208.

”Hybrid Polymer/Metal-Organic Framework Films for Colorimetric Water Sensing over a Wide Concentration Range”

1. Skripov, A. V.; Skoryunov, R. V.; Soloninin, A. V.; Babanova, O. A.; Stavila, V.; Udovic, T. J. *Journal of Physical Chemistry C* **2018,** *122*, 3256-3262.

”Nuclear Magnetic Resonance Study of Anion and Cation Reorientational Dynamics in (NH4)2B12H12”

1. Wood, B. C.; Stavila, V.; Poonyayant, N.; Heo, T. W.; Ray, K. G.; Klebanoff, L. E.; Udovic, T. J.; Lee, J. R. I.; Angboonpong, N.; Sugar, J. D.; Pakawatpanurut, P., *Advanced Materials Interfaces* **2017,** *4*, 1300803.

“Nanointerface-Driven Reversible Hydrogen Storage in the Nanoconfined Li-N-H System”

1. Tang, W. S.; Dimitrievska, M.; Stavila, V.; Zhou, W.; Wu, H.; Talin, A. A.; Udovic, T. J., *Chemistry of Materials* **2017,** *29*, 10496-10509.

“Order-Disorder Transitions and Superionic Conductivity in the Sodium nido-Undeca(carba)borates”

1. Varley, J. B.; Kweon, K.; Mehta, P.; Shea, P.; Heo, T. W.; Udovic, T. J.; Stavila, V.; Wood, B. C., *ACS Energy Letters* **2017,** *2*, 250-255.

“Understanding Ionic Conductivity Trends in Polyborane Solid Electrolytes from Ab Initio Molecular Dynamics”

1. Spoerke, E. D.; Small, L. J.; Foster, M. E.; Wheeler, J.; Ullman, A. M.; Stavila, V.; Rodriguez, M.; Allendorf, M. D. *Journal of Physical Chemistry C* **2017,** *121*, 4816-4824

“MOF-Sensitized Solar Cells Enabled by a Pillared Porphyrin Framework”

1. Kweon, K. E.; Varley, J. B.; Shea, P.; Adelstein, N.; Mehta, P.; Heo, T. W.; Udovic, T. J.; Stavila, V.; Wood, B. C. *Chemistry of Materials* **2017,** *29*, 9142-9153.

“Structural, Chemical, and Dynamical Frustration: Origins of Superionic Conductivity in closo-Borate Solid Electrolytes”

1. Bukovsky, E. V.; Peryshkov, D. V.; Wu, H.; Zhou, W.; Tang, W. S.; Jones, W. M.; Stavila, V.; Udovic, T. J.; Strauss, S. H. *Inorganic Chemistry* **2017,** *56*, 4369-4379.

“Comparison of the Coordination of B12F122-, B12Cl122-, and B12H122- to Na+ in the Solid State: Crystal Structures and Thermal Behavior of Na2(B12F12), Na2(H2O)4(B12F12), Na2(B12Cl12), and Na2(H2O)6(B12Cl12)”

1. Chae, J.; An, S.; Ramer, G.; Stavila, V.; Holland, G.; Yoon, Y.; Talin, A. A.; Allendorf, M.; Aksyuk, V. A.; Centrone, A. *Nano Letters* **2017,** *17*, 5587-5594.

“Nanophotonic Atomic Force Microscope Transducers Enable Chemical Composition and Thermal Conductivity Measurements at the Nanoscale”

1. Dolgopolova, E. A.; Brandt, A. J.; Ejegbavwo, O. A.; Duke, A. S.; Maddumapatabandi, T. D.; Galhenage, R. P.; Larson, B. W.; Reid, O. G.; Ammal, S. C.; Heyden, A.; Chandrashekhar, M.; Stavila, V.; Chen, D. A.; Shustova, N. B. *Journal of the American Chemical Society* **2017,** *139*, 5201-5209.

“Electronic Properties of Bimetallic Metal-Organic Frameworks (MOFs): Tailoring the Density of Electronic States through MOF Modularity”

1. Soloninin, A. V.; Dimitrievska, M.; Skoryunov, R. V.; Babanova, O. A.; Skripov, A. V.; Tang, W. S.; Stavila, V.; Orimo, S.; Udovic, T. J. *Journal of Physical Chemistry C* **2017,** *121*, 1000-1012. “Comparison of Anion Reorientational Dynamics in MCB9H10 and M2B10H10 (M = Li, Na) via Nuclear Magnetic Resonance and Quasielastic Neutron Scattering Studies”
2. Perez-Pimienta, J. A.; Sathitsuksanoh, N.; Thompson, V. S.; Tran, K.; Ponce-Noyola, T.; Stavila, V.; Singh, S.; Simmons, B. A. *Biotechnology for Biofuels,* **2017**, *10,* 72.

“Ternary ionic liquid-water pretreatment systems of an agave bagasse and municipal solid waste blend”

1. Ray, K. G.; Klebanoff, L. E.; Lee, J. R. I.; Stavila, V.; Heo, T. W.; Shea, P.; Baker, A. A.; Kang, S.; Bagge-Hansen, M.; Liu, Y. S.; White, J. L.; Wood, B. C., *Physical Chemistry Chemical Physics,* **2017**, *19,* 22646-22658.

“Elucidating the mechanism of MgB2 initial hydrogenation via a combined experimental-theoretical study”

1. V. Stavila, R. Parthasarathi, R.W. Davis, F. El Gabaly, K.L. Sale, B.A. Simmons, S. Singh, M.D. Allendorf, *ACS Catalysis,* **2016**, *6,* 55-59.

“MOF-Based Catalysts for Selective Hydrogenolysis of Carbon–Oxygen Ether Bonds”

1. V. Stavila, C. Schneider, C. Mowry, T. R. Zeitler, J.A. Greathouse, A.L. Robinson, J.M. Denning, J. Volponi, K. Leong, W. Quan, M. Tu, R.A. Fischer, M.D. Allendorf, *Advanced Functional Materials,* **2016**, *26*, 1699-1707.

“Thin film growth of nbo MOFs and their integration with electroacoustic devices”

1. M.D Allendorf, V. Stavila, *Nature Materials,* **2016**, *15*, 255-257.

“Nanoporous films: From conventional to conformal”

1. J. L. White, R. J. Newhouse, J. Z. Zhang, T. J. Udovic, V. Stavila, *Journal of Physical Chemistry* *C,* **2016**, *120,* 25725-25731.

“Understanding and mitigating the effects of stable dodecahydro-*closo*-dodecaborate intermediates of hydrogen storage reactions”

1. Dimitrievska, M.; White, J. L.; Zhou, W.; Stavila, V.; Klebanoff, L. E.; Udovic, T. J. *Physical Chemistry Chemical Physics,* **2016**, *18,* 25546-25552.

“Structure-dependent vibrational dynamics of Mg(BH4)2 polymorphs probed with neutron vibrational spectroscopy and first-principles calculations”

1. Jones, C. G.; Stavila, V.; Conroy, M. A.; Feng, P.; Slaughter, B. V.; Ashley, C. E.; Allendorf, M. D., *ACS Applied Materials & Interfaces,* **2016**, *8,* 7623-7630.

“Versatile Synthesis and Fluorescent Labeling of ZIF-90 Nanoparticles for Biomedical Applications”

1. X. Zhou, F. El Gabaly, V. Stavila, M. D. Allendorf, *Journal of Physical Chemistry* *C,* **2016**, *120,* 7500-7509.

“Molecular dynamics simulations of hydrogen diffusion in aluminum”

1. W. S. Tang, M. Matsuo, H. Wu, V. Stavila, W. Zhou, A. A. Talin, A. V. Soloninin, R. V. Skoryunov, O. A. Babanova, A. V. Skripov, S. Orimo, T. J. Udovic, *Advanced Energy Materials,* **2016**, *6,* 1502237.

“Liquid-like ionic conduction in solid lithium and sodium monocarba-*closo*-decaboranes near or at room temperature”

1. W. S. Tang, K. Yoshida, A. V. Soloninin, R. V. Skoryunov, O. A. Babanova, A. V. Skripov, M. Dimitrievska, V. Stavila, S. Orimo, T. J. Udovic, *ACS Energy Letters,* **2016**, *1,* 659-664.

“Stabilizing superionic-conducting structures via mixed-anion solid solutions of monocarba-*closo*-borate salts”

1. Perez-Pimienta, J. A.; Poggi-Varaldo, H. M.; Ponce-Noyola, T.; Ramos-Valdivia, A. C.; Chavez-Carvayar, J. A.; Stavila, V.; Simmons, B. A., *Biomass & Bioenergy,* **2016**, *91,* 48-55.

“Fractional pretreatment of raw and calcium oxalate-extracted agave bagasse using ionic liquid and alkaline hydrogen peroxide”

1. Wu, H.; Tang, W. S.; Zhou, W.; Tarver, J. D.; Stavila, V.; Brown, C. M.; Udovic, T. J. *Journal of Solid State Chemistry,* **2016**, *243,* 162-167.

“The low-temperature structural behavior of sodium 1-carba-closo-decaborate: NaCB9H10”

1. Ullman, A. M.; Brown, J. W.; Foster, M. E.; Leonard, F.; Leong, K.; Stavila, V.; Allendorf, M. D. *Inorganic Chemistry,* **2016**, *55,* 7233-7249.

“Transforming MOFs for Energy Applications Using the Guest@MOF Concept”

1. R.L. Davidovich, D.V. Marinin, V. Stavila, K.H. Whitmire,  *Coordination Chemistry Reviews*, **2015**,*299*, 61-82.

“Structural chemistry of fluoride and oxofluoride complexes of titanium (IV)”

1. A. Unemoto, T. Ikeshoji, S. Yasaku, M. Matsuo, V. Stavila, T.J. Udovic, S. Orimo, *Chemistry of Materials,* **2015**, *27,* 5407-5416.

“Stable interface formation between TiS2 and LiBH4 in bulk-type all-solid-state lithium batteries”

1. M.D. Allendorf, V. Stavila, *CrystEngComm,* **2015**, *17,* 229–246.

“Crystal engineering, structure-function relationships, and the future of metal-organic frameworks”

1. W.S. Tang, A. Unemoto, W. Zhou, V. Stavila, M. Matsuo, H. Wu, S. Orimo, T.J. Udovic, *Energy and Environmental Science,* **2015**, *8,* 3637-3645.

“Unparalleled lithium and sodium superionic conduction in solid electrolytes with large monovalent cage-like anions”

1. H. Wu, W.S. Tang, W. Zhou, V. Stavila, J.J.Rush, T.J. Udovic, *CrystEngComm,* **2015**, *17,* 3533-3540.

“The structure of monoclinic Na2B10H10: a combined diffraction, spectroscopy, and theoretical approach”

1. N. Yang, J.K. Yee, Z. Zhang, C. San Marchi, V. Stavila, E. Lavernia, *Acta Materialia,* **2015**, *82,* 41-50.

“Hydrogen sorption characteristics of nanostructured Pd-10Rh processed by cryomilling”

1. K.J. Erickson, F. Léonard, V. Stavila, M.E. Foster, C.D. Spataru, R.E. Jones, B.M. Foley, P.E. Hopkins, M.D. Allendorf, A.A. Talin, *Advanced Materials,* **2015**, *27,* 3453-3459.

“Thin film thermoelectric Metal–Organic Framework with high Seebeck coefficient and low thermal conductivity”

1. K.R. Reyes-Gil, Z.D. Stephens, V. Stavila, D.B. Robinson, *ACS Applied Materials & Interfaces,* **2015**, *7,* 2202-2213.

“Composite WO3/TiO2 nanostructures with high electrochromic activity”

1. A.V. Skripov, R.V. Skoryunov, A.V. Soloninin, O.A. Babanova, W.S. Tang, V. Stavila, T.J. Udovic, *Journal of Physical Chemistry C*,**2015**, *119*, 26912-26918.

“Anion Reorientations and Cation Diffusion in LiCB11H12 and NaCB11H12: 1H, 7Li, and 23Na NMR Studies”

1. M.D. Allendorf, M.E. Foster, F. Léonard, V. Stavila, P.L Feng, P. Doty, K. Leong, E.Y. Ma, S.R. Johnson, *The Journal of Physical Chemistry Letters,* **2015**, *6,* 1182-1195.

“Thin film thermoelectric Metal–Organic Framework with high Seebeck coefficient and low thermal conductivity”

1. H. Wu, W.S. Tang, V. Stavila, W. Zhou, J.J. Rush, T.J. Udovic, *Journal of Physical Chemistry C*,**2015**, *119*, 6481-6487.

“Structural Behavior of Li2B10H10”

1. W.S. Tang, T.J. Udovic, V. Stavila, *Journal of Alloys and Compounds*,**2015**, *645*, S200-S204. “Altering the structural properties of A2B12H12 compounds via cation and anion modifications”
2. C. Scullin, V. Stavila, A. Skarsdad, D.Y. Xu, J. Mentel, B.A. Simmons, S. Singh, *Bioresource Technology,* **2015**, *184,* 415-420.

“Optimization of renewable pipene production from the conversion of microalgae *Saccharina Latissima*”

1. J. Shi, K.W. George, N. Sun, W. He, C. Li, V. Stavila, J.D. Keasling, B.A. Simmons, S. Singh, *Bioenergy Research,* **2015**, *8,* 1004-1013.

“Impact of pretreatment technologies on saccharification and isopentenol fermentation of mixed lignocellulosic feedstocks”

1. A. George, A. Brandt, K. Tran, S.M.S. Zahari, D. Klein-Marcuschamer, J. Shi, V. Stavila, R. Parthasarathi, S. Singh, B.M Holmes, T. Welton, B.A. Simmons, J.P. Hallett, *Green Chemistry,* **2015**, *17,* 1728-1734.

“Design of low-cost ionic liquids for lignocellulosic biomass pretreatment”

1. J.A. Perez-Pimienta, M.G. Lopez-Ortega, J.A. Chavez-Carvayar, P. Varanasi, V. Stavila, A. G. Cheng, S. Singh, B.A. Simmons, *Biomass and Bioenergy,* **2015**, *75,* 180-188.

“Characterization of agave bagasse as a function of ionic liquid pretreatment”

1. V. Stavila, A.A. Talin, M.D. Allendorf, *Chemical Society Reviews,* **2014**, *43,* 5994-6010.

“MOF-based electronic and opto-electronic devices”

1. A.A. Talin, A. Centrone, A.C. Ford, M.E. Foster, V. Stavila, P. Haney, R.A. Kinney, V. Szalai, F. El Gabaly, H.P. Yoon, F. Leonard, M.D. Allendorf, *Science,* **2014**, *343,* 66–69.

“Tunable electrical conductivity in Metal-Organic Framework thin-film devices”

1. P.A. Sharma, A.L. Lima, M. Heckmaty, V. Stavila, D. Medlin, *Applied Physics Letters,* **2014**, *105,* 242106.

“Ion beam modification of topological insulator bismuth selenide”

1. T.J. Udovic, M. Matsuo, A. Unemoto, N. Verdal, V. Stavila, A.V. Skripov, J.J. Rush, H. Takamure, S. Orimo, *Chemical Communications,* **2014**, *50,* 3750-3752.

“Sodium superionic conduction in Na2B12H12”

1. T.J. Udovic, M. Matsuo, W.S. Tang, A. Unemoto, N. Verdal, V. Stavila, A.V. Skripov, J.J. Rush, H. Takamure, S. Orimo, *Advanced Materials,* **2014**, *26,* 7622-7626.

“Exceptional superionic conductivity in disordered sodium decahydro-*closo*-decaborate”

1. N. Verdal, T.J. Udovic, V. Stavila, A.V. Skripov, J.J. Rush, *Journal of Physical Chemistry* *C*, **2014**, *118*, 17483–17489.

“Anion reorientations in the superionic conducting phase of Na2B12H12”

1. N. Poonyayant, V. Stavila, E.H. Majzoub, M. Ulutagay-Kartin, L.E. Klebanoff, *Journal of Physical Chemistry* *C*, **2014**, *118*, 14759–14769.

“An investigation into hydrogen storage characteristics of Ca(BH4)2/LiNH2 and Ca(BH4)2/NaNH2: Evidence of intramolecular destabilization”

1. C.G. Jones, P.J. Cappillino, V. Stavila, D.B. Robinson, *Powder Technology,* **2014**, *267,* 95-102.

“Control of both particle and pore size in nanoporous palladium alloy powders”

1. R.L. Davidovich, V.V. Tkachev, V.B. Logvinova, V. Stavila, *Journal of Structural Chemistry,* **2014**, *55,* 1083-1090.

“New structure types of polymeric chain anions in the crystal structures of complex zirconium fluorides”

1. N. Sathitsuksanoh, K.M. Holtman, D.J. Yelle, T. Morgan, V. Stavila, J. Pelton, H. Blanch, B.A. Simmons, A. George, *Green Chemistry,* **2014**, *16,* 1236-1247.

“Lignin fate and characterization during ionic liquid biomass pretreatment for renewable chemicals and fuels production”

1. M.J. Dougherty, H.M. Tran, V. Stavila, B. Knierim, A. George, M. Auer, P.D. Adams, M.Z. Hadi, *Plos One,* **2014**, *9,* e100836.

“Cellulosic Biomass Pretreatment and Sugar Yields as a Function of Biomass Particle Size”

1. N. Verdal, J.-H. Her, V. Stavila, A.V. Soloninin, O.A. Babanova, A.V. Skripov, T.J. Udovic, J.J. Rush, *Journal of Solid State Chemistry,* **2014**, *212,* 81-91.

“Complex high-temperature phase transitions in Li2B12H12 and Na2B12H12”

1. N. Sun, R. Parthasarathi, A.M. Socha, J. Shi, S. Zhang, V. Stavila, K.L. Sale, B.A. Simmons, S. Singh, *Green Chemistry,* **2014**, *16,* 2546-2557.

“Understanding pretreatment efficacy of four cholinium and imidazolium ionic liquids by chemistry and computation”

1. A.M. Socha, R. Parthasarathi, J. Shi, V. Stavila, D.Y. Xu, J. Mentel, B.A. Simmons, S. Singh, *Proceedings of the National Academy of Sciences,* **2014**, *111,* E3587-E3595.

“Efficient biomass pretreatment using ionic liquids derived from lignin and hemicellulose”

1. J. Shi, K. Balamurugan, R. Parthasarathi, V. Stavila, J. Mentel, B.A. Simmons, S. Singh, *Green Chemistry,* **2014**, *16,* 3830-3840.

“Understanding the role of water during ionic liquid pretreatment of lignocellulose: co-solvent or anti-solvent?”

1. V. Stavila, D.B. Robinson, Hekmaty M.A, R. Nishimoto, D.L. Medlin, S. Zhu, T.M. Tritt, P.A. Sharma, *ACS Applied Materials & Interfaces*,**2013**, *5,* 6678–6686.

“Wet-chemical synthesis and consolidation of stoichiometric bismuth telluride nanoparticles for improving the thermoelectric figure-of-merit”

1. X. Liu, E.H. Majzoub, V. Stavila, R. Bhakta, M.D. Allendorf, M. Conradi, N. Verdal, T. Udovic, *Journal of Materials Chemistry A*,**2013**, *1,* 9935-9941.

“Probing the unusual anion mobility of LiBH4 confined in highly ordered nanoporous carbon frameworks via solid state NMR and quasielastic neutron scattering”

1. I. Ellern, A. Vankatasubramanian, J.H. Lee, P.J. Hesketh, V. Stavila, A. Robinson, M.D. Allendorf, *Micro and Nano Letters,* **2013**, *8,* 766–769.

“HKUST-1 coated piezoresistive microcantilever array for volatile organic compound sensing”

1. A.V. Skripov, O.A. Babanova, A.V. Soloninin, V. Stavila, N. Verdal, T.J. Udovic, J.J. Rush, *Journal of Physical Chemistry C*,**2013**, *117,* 25961-25968.

“Nuclear magnetic resonance study of atomic motion in A2B12H12 (A = Na, K, Rb, Cs): Anion reorientations and Na+ mobility”

1. P.J. Cappillino, K.M. Hattar, B.G. Clark, V. Stavila, J. Sugar, D.B. Robinson, *Journal of Materials Chemistry A*,**2013**, *1,* 602-610.

“Synthesis of mesoporous palladium with tunable porosity and demonstration of its thermal stability by *in situ* heating and environmental transmission electron microscopy”

1. R.L. Davidovich, D.V. Marinin, V. Stavila, K.H. Whitmire,  *Coordination Chemistry Reviews*, **2013**,*257*, 3074–3088.

“Stereochemistry of fluoride and mixed-fluoride complexes of zirconium and hafnium”

1. A. Eichorst, P. Varanasi, V. Stavila, M. Zemla, M. Auer, S. Singh, B.A. Simmons, *Environmental Microbiology* **2013**, *15,* 2573-2587.

“Community dynamics of cellulose-adapted thermophilic bacterial consortia”

1. A.M. Socha, S.P. Plummer, V. Stavila, B.A. Simmons, S. Singh, *Biotechnology for Biofuels*,**2013**, *6,* 61.

“Comparison of content for ionic liquid pretreated Douglas-fir woodchips and forestry residues”

1. A.G. Cruz, C. Scullin, C. Mu, G. Cheng, V. Stavila, P. Varanasi, D.Y. Xu, J. Mentel, Y.D. Chuang, B.A. Simmons, S. Singh, *Biotechnology for Biofuels*,**2013**, *6,* 52, DOI: 10.1186/1754-6834-6-52.

“Impact of high biomass loading on ionic liquid pretreatment”

1. N. Sun, H. Liu, N. Sathitsuksanoh, A. George, V. Stavila, B.A. Simmons, S. Singh, *Biotechnology for Biofuels*,**2013**, *6,* 1-15.

“Production and extraction of sugars from switchgrass hydrolyzed in ionic liquids”

1. J.A. Perez-Pimienta, M.G. Lopez-Ortega, P. Varanasi, C. Scullin, G. Cheng, V. Stavila, B.A. Simmons, S. Singh, *Bioresource Technology*,**2013**, *127,* 18-24.

“Comparison of the impact of ionic liquid pretreatment on recalcitrance of agave bagasse and switchgrass”

1. J. Shi, V.S. Thompson, N.A. Yancey, V. Stavila, B.A. Simmons, S. Singh, *Biofuels*,**2013**, *4,* 63-72.

“Impact of mixed feedstocks and feedstock densification on ionic liquid pretreatment efficiency”

1. V. Stavila, R.K. Bhakta, T.M. Alam, E.H. Majzoub, M.D. Allendorf, *ACS Nano,* **2012**, *6,* 9807-9817.

“Reversible Hydrogen Storage by NaAlH4 Confined within a Titanium-Functionalyzed MOF-74(Mg) Nanoreactor”

1. G. Cheng, P. Varanasi, R. Arora, C. Scullin, V. Stavila, B.A. Simmons, S. Singh, *Journal of Physical Chemistry B*,**2012**, *116,* 10049-10054.

“Impact of ionic liquid pretreatment conditions on cellulose crystalline structure using 1-ethyl-3-methylimidazolium acetate”

1. H. Liu, G. Cheng, M. Kent, P. Varanasi, V. Stavila, B.A. Simmons, S. Singh, *Journal of Physical Chemistry B,* **2012**, *116,* 8131–8138.

“Simulations reveal conformational changes of methylhydroxyl groups during dissolution of cellulose *Ibeta* in ionic liquid 1-ehtyl-3-methyl-imidazolinium acetate”

1. V. Stavila, J. Volponi, A.M. Katzenmeyer, M.C. Dixon, M.D. Allendorf, *Chemical Science,* **2012**, *3,* 1531–1540.

“Kinetics and mechanism of Metal-Organic Frameworks thin film growth: Systematic investigation of HKUST-1 deposition on QCM electrodes”

1. A.L. Robinson, V. Stavila, T.R. Zeitler, M.I. White, S.M. Thornberg, J.A. Greathouse, M.D. Allendorf, *Analytical Chemistry,* **2012**, *84*, 7043-7051.

“Ultrasensitive humidity detection using Metal-Organic Framework-coated microsensors”

1. A. Vankatasubramanian, J.H. Lee, V. Stavila, A. Robinson, M.D. Allendorf, P.J. Hesketh, *Sensors and Actuators B: Chemical,* **2012**, *168,* 256–262.

“MOF@MEMS: Design Optimization for High Sensitivity Chemical Detection”

1. R.K. Bhakta, S. Maharrey, V. Stavila, E.H. Majzoub, M.D. Allendorf, *Physical Chemistry Chemical Physics,* **2012**, *14,* 8160–8169.

“Thermodynamics and Kinetics of NaAlH4 Nanocluster Decomposition”

1. D. Banga, J.L. Lensch-Falk, D.L. Medlin, V. Stavila, N.Y.C. Yang, D.B. Robinson, P.A. Sharma, *Crystal Growth & Design,* **2012**, *12*, 1347–1353.

“Periodic Modulation of Sb Stoichiometry in Bi2Te3/Bi2-xSbxTe3 Multilayers Using Pulsed Electrodeposition”

1. J.L. Lensch-Falk, D. Banga, P.E. Hopkins, D.B. Robinson, V. Stavila, P.A. Sharma, D.L. Medlin, *Thin Solid Films,* **2012**, *520*, 6109–6117.

“Electrodeposition and characterization of nanocrystalline antimony telluride thin films”

1. P.J. Cappillino, J.D. Sugar, M.A. Hekmaty, B.W. Jacobs, V. Stavila, P.G. Kotula, J.M. Chames, N.Y. Yang, D.B. Robinson, *Journal of Materials Chemistry*, **2012**,*22*, 14013–14022.

“Nanoporous Pd alloys with compositionally tunable hydrogen storage properties prepared by nanoparticle consolidation”

1. J.H. Her, H. Wu, N. Verdal, W. Zhou, V. Stavila, T.J. Udovic, *Journal of Alloys and Compounds,* **2012**, *514,* 71–75.

“Structures of strontium and darium dodecahydro-*closo*-dodecaborates”

1. G. Papa, P. Varanasi, L. Sun, G. Cheng, V. Stavila, B. Holmes, B.A. Simmons, F. Adani, S. Singh, *Bioresource Technology,* **2012**, *117*, 352–359.

“Exploring the effect of different plant lignin content and composition on ionic liquid pretreatment efficiency and enzymatic sacharification of *Eucalyptus Globulus L.* mutants”

1. W. Luo, V. Stavila, L.E. Klebanoff, *International Journal of Hydrogen Energy,* **2012**, *37,* 6646–6652.

“New insights into the mechanism of activation and hydrogen absorption of (2LiNH2-MgH2)”

1. M.D. Allendorf, A. Schwartzberg, V. Stavila, A.A. Talin, *Chemistry – A European Journal,* **2011**, *17,* 11372–11288.

“A roadmap to implementing Metal-Organic Frameworks in electronic devices: Challenges and critical directions”

1. M.P. Klein, B.W. Jacobs, M.D. Ong, S.J. Fares, D.B. Robinson, V. Stavila, G.J. Wagner, I. Arslan, *Journal of the American Chemical Society*, **2011**,*133*, 9144–9147.

“Three-dimensional pore evolution of nanoporous metal particles for energy storage”

1. N. Verdal, W. Zhou, V. Stavila, J.-H. Her, M. Yousufuddin, T. Yildirim,T.J. Udovic, *Journal of Alloys and Compounds*, **2011**, *509*, S694-S697.

“Alkali and Alkali-Earth Metal Dodecahydro-*Closo*-Dodecaborates: Probing Structural Variations *via* Neutron Vibrational Spectroscopy”

1. N. Verdal, H. Wu, T.J. Udovic, V. Stavila, W. Zhou, J.J. Rush, T.J. Udovic. *Journal of Solid State Chemistry*, **2011**,*184*, 3110–3116.

“Evidence of a transition to reorientational disorder in the cubic alkali-metal dodecahydro-*closo*-dodecaborates”

1. N. Verdal, T.J. Udovic, J.J. Rush, V. Stavila, H. Wu, W. Zhou, T. Jenkins, *Journal of Chemical Physics*, **2011**,*135*, 094501.

“Low-temperature tunneling and rotational dynamics of the ammonium cations in (NH4)2B12H12”

1. D.T. Shane, L.H. Rayhel, Z.G. Huang, J.C. Zhao, X. Tang, V. Stavila, M.S. Conradi, *Journal of Physical Chemistry C,* **2011**, *115,* 3172–3177.

“Comprehensive NMR Study of Magnesium Borohydrdie”

1. V. Stavila, J.-H. Her, W. Zhou, S.-J. Hwang, Ch. Kim, L.-A. M. Ottley, T.J. Udovic, *Journal of Solid State Chemistry,* **2010**, *183,* 1133–1140.

“Calcium Dodecahydro-*closo*-dodecaborate: Synthesis, Structure and Relevance to Hydrogen Storage”

1. V. Stavila, I. Bulimestru, A. Gulea, A.C. Colson, K.H. Whitmire., *Acta Crystallographica, Section C,*  **2011**, *C67*, m65-m68.

“Hexaaquacobalt(II) and Hexaaquanickel(II) *bis*(μ-pyridine-2,6-dicarboxylato)*bis*[(pyridine-2,6-dicarboxylato) bismuthate(III)] Dihydrate”

1. V. Stavila, K.H. Whitmire., *Acta Crystallographica, Section E,*  **2010**, *E66*, m1547-m1548.

“(N,N-Dimethylformamide-*κO*)bis(3-hydroxypicolinato-*κ2N,O2*)phenylbismuth(III)”

1. T. Mandal, G. Piburn, V. Stavila, I. Rusakova, T. Ould-Ely, A.C. Colson, K.H. Whitmire, *Chemistry of Materials*, **2011**, *23*, 4158–4169.

“New Mixed Ligand Single-Source Precursors for PbS Nanoparticles and Their Solvothermal Decomposition to Anisotropic Nano- and Microstructures”

1. R. Newhouse, V. Stavila, S. Hwang, L.E. Klebanoff, J. Zhang, *Journal of Physical Chemistry* *C*, **2010**, *114*, 5224–5232.

“Reversibility and Improved Hydrogen Release of Magnesium Borohydride”

1. W. Luo, D. Cowgill, K. Stewart, V. Stavila, *Journal of Alloys and Compounds,* **2010**, *497,* L17–L20.

“High Capacity Hydrogen Generation on Demand from (NH3 + LiAlH4)”

1. K.C. Kim, M.D. Allendorf, V. Stavila, D.S. Sholl, *Physical Chemistry Chemical Physics,* **2010**, *12*, 9918–9926.

“Predicting Impurity Gases and Phases during Hydrogen Evolution from Complex Metal Hydrides Using Free Energy Minimization Enabled by First-Principles Calculations”

1. R.L. Davidovich, V. Stavila, K.H. Whitmire,  *Coordination Chemistry Reviews*, **2010**,*250*, 2782–2810.

“Stereochemistry of Lead(II) Complexes Containing Sulfur and Selenium Donor Atom Ligands”

1. V. Stavila, I. Rusakova, K.H. Whitmire, *Chemistry of Materials*, **2009**, *21*, 5456–5465.

“Synthesis of Bi2S3 Nanostructures from Bismuth(III) Thiourea and Thiosemicarbazide Complexes”

1. T. Mandal, V. Stavila, I. Rusakova, S. Ghosh, K.H. Whitmire, *Chemistry of Materials*, **2009**, *21*, 5617–5626.

“Molecular Precursors for CdS Nanoparticles: Synthesis and Characterization of Carboxylate-Thiourea or –Thiosemicarbazide Cadmium Complexes and Their Decomposition”

1. J.-H. Her, W. Zhou, V. Stavila, C.M. Brown,T.J. Udovic, *Journal of Physical Chemistry*, C, **2009**, *113*, 11187–11189.

“The Crystal Structure of Na2B12H12 and the Role of Cation Size on the Structural Behavior of the Alkali-Metal Dodecahydro-*closo*-dodecaborates”

1. R.L. Davidovich, V. Stavila, D.V. Marinin, E.I. Voit, K.H. Whitmire,  *Coordination Chemistry Reviews*, **2009**,*253*, 1316–1352.

“Stereochemistry of Lead(II) Complexes with Oxygen Donor Ligands”

1. V. Stavila, E. Dikarev,  *Journal of Organometallic Chemistry*, **2009**,*694*, 2956–2964.

“Phenyl Bismuth *Beta*-Diketonate Complexes: Synthesis and Structural Characterization”

1. V. Stavila, J.H. Thurston, K.H. Whitmire, *Inorganic Chemistry*,**2009**, *48*, 6945–6951.

“Selective Arylation Reactions of Bismuth-Transition Metal Salicylate Complexes”

1. V. Stavila, Y. Stortz, C. Franc, D. Pitrat, P. Maurin, J. Hasserodt, *European Journal of Inorganic Chemistry*, **2008**, 3943–3947.

“**Effective Repression of the Fragmentation of a Hexadentate Ligand Bearing an Auto-Immolable Pendant Arm by Iron Coordination**”

1. V. Stavila, M. Allali, L. Canaple, Y. Stortz, C. Franc, P. Maurin, O. Beuf, O. Dufay, J. Samarut, M. Janier, J. Hasserodt, *New Journal of Chemistry*, **2008,** *32,* 428–435*.*

“Significant Relaxivity Gap Between a Low-Spin and a High-Spin Iron(II) Complex of Structural Similarity: An Attractive Off-On System for the Potential Design of Responsive MRI Probes”

1. A. Gulea, D. Poirier, J. Roy, V. Stavila, I. Bulimestru, V. Tapcov, M. Birca, L. Popovschi, *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2008**, *23*, 806–818.

“**In vitro antileukemia, antibacterial and antifungal activities of some 3d metal complexes: Chemical synthesis and structure – activity relationships**”

1. P. Maurin, V. Stavila, M. Allali, L. Canaple, O. Beuf, Y. Stortz, J. Samarut, M. Janier, J. Hasserodt, *Bulletin du Cancer*, **2008,** *95,* S24–S25*.*

“Studies regarding the adjustment of bioactivatable contrast agents with an iron base for *in vivo* MRI”

1. V. Stavila, J.H. Thurston, D. Prieto-Centurion, K.H. Whitmire, *Organometallics,* **2007**, *26*, 6864–6866.

 “A new methodology for synthesis of aryl bismuth compounds: Arylation of bismuth(III) carboxylates by sodium tetraarylborate salts*”*

1. V. Stavila, J.C. Fettinger, K.H. Whitmire, *Organometallics,* **2007**, *26*, 3321–3328.

“Synthesis and characterization of new phenylbis(salicylato)-bismuth(III) complexes*”*

1. V. Stavila, R.L. Davidovich, A. Gulea, K.W. Whitmire, *Coordination Chemistry Reviews*, **2006,** *250,* 2782–2810*.*

“Bismuth(III) complexes with aminopolycarboxylate and polyaminopolycarboxylate ligands: Chemistry and structure”

1. I.G. Filippova, Yu.A. Simonov, M. Gdanets, V. Stavila, *Journal of Structural Chemistry*, **2005,** *46*, 1095–1098.

“Crystal structure of *tris*(1,10-phenanthroline) iron(II) dinitrate dihydrate”

1. V. Stavila, A. Gulea, S. Shova, Yu.A. Simonov, P. Petrenko, J. Lipkowski, F. Riblet, L. Helm, *Inorganica Chimica Acta*, **2004**, *357*. 2060–2068.

“An unexpected influence of the nature of the amine on the crystal structure of some Co(III)-Bi(III) heterometallic complexes*”*

1. V. Stavila, A. Gulea, N. Popa, S. Shova, A. Merbach, Yu.A. Simonov, J. Lipkowski, *Inorganic Chemistry Communications*,**2004**, *7*, 634–637.

“A novel 3D Nd(III)-Bi(III) coordination polymer generated from EDTA ligand”

1. P. A. Petrenko, M. Gdaniec, Yu. A. Simonov, V. Stavila, A. Gulea. *Russian Journal of Coordination Chemistry*,**2004**, *30*, 813–817.

“Crystal Structure of Monoprotonated Ni(II) Nitrilotriacetate Tetrahydrate”

1. V. Stavila, J.-P. Wignacourt, E. Holt, P. Conflant, M. Drache, A. Gulea. . *Inorganica Chimica Acta*, **2003**, *353*, 43–50.

“Synthesis and Structure of Some Co(III)-Bi(III) Complexes: [Co(NH3)5NCS][Bi(Edta)]2⋅4H2O, [Co(NH3)4(NO2)2][Bi(Edta)(H2O)]⋅2H2O, and [Co(NH3)4CO3](BiEdta)⋅3H2O”

1. R. Bachman, K. Whitmire, J. Thurston, A. Gulea, O. Stavila, V. Stavila. *Inorganica Chimica Acta*, **2003**, *346*, 249–255.

“Bismuth Ladder Polymers: Structural and Thermal Studies of [Bi(OCH2CH2)3N]n and [(BixTb1-x(O2C2H2)3N)·2H2O]n”

1. V. Stavila, A. Gulea, S. Shova, M. Gdanec, Yu.A. Simonov. *Russian Journal of Coordination Chemistry*,**2002**, *28*, 565–572.

“Synthesis and Study of Heterometallic Co-Bi Compounds Based on Ethylenediaminetetraacetic Acid. Crystal and Molecular Structures of [Co(DH)2(2-NH2C6H4CH3)2]2[Bi2(μ-Edta)2(H2O)2]·10H2O”

1. V. Stavila, M. Gdanec, S. Shova, Yu.A. Simonov, A. Gulea, J.-P. Wignacourt, *Russian Journal of Coordination Chemistry*,**2000**, *26*, 741–747.

“Synthesis and structure of {μ-oxalato-bis[(ethylenediaminetetraacetato)-bismuthate(III)]} pentaamminethiocyanatocobalt(III)dodecahydrate, [Co(NH3)5NCS]2[(EDTA)Bi(μ-C2O4)Bi(EDTA)]·12H2O”

**Patents**

1. M.D. Allendorf, A.A. Talin, F. Leonard, V. Stavila, *US Patent # 9711743 granted on 07/18/2018* (**2018**).

“Reconfigurable Electronics Using Conducting Metal-Organic Frameworks”

1. V. Stavila, L.E. Klebanoff, *US Patent # 10000377 granted on 06/19/2018* (**2018**).

“Nanostructured Metal Amides and Nitrides for Hydrogen Storage”

1. V. Stavila, L.E. Klebanoff, *US Patent Application # 15/812254* (**2017**).

“Ternary Borides and Borohydrides for Hydrogen Storage and Method of Synthesis”

1. V. Stavila, J.L. White, *US Patent Application # 16/000,683* (**2016**).

“Solid state synthesis of metal borohydrides”

1. M.D. Allendorf, F. Leonard, A.A. Talin, V. Stavila, *US Patent # 9428525 granted on 8/30/2016* (**2016**)

 “Tunable Electrical Conductivity in Metal-Organic Framework Thin Film Devices”

1. M.D. Allendorf, V. Stavila, *US Patent Application # 14/991734* (**2014**).

“Metal-Organic Framework Catalysts for Selective Cleavage of Aryl-Ether Bonds”

1. M.D. Allendorf, A.A. Talin, F. Leonard, V. Stavila, *US Patent Application # 14/573990* (**2014**).

“Multiaxis Sensing Using Electrically Conductive Metal-Organic Frameworks”

1. S. Baranov, B. Cinic, I. Redwing, Vitalie Stavila, *Moldovan Patent MD-2937* (**2006**).

“Process for Cleaning Machining Attachments from Waste after Epitaxial Growth of Semiconductor Layers”

1. A. Gulea, A. Cecal, A. Paraschivescu, V. Stavila, V. Tapcov, N. Popa, *Moldovan Patent MD-2673* (**2005**).

“Lanthanum Bismuthate as Catalyst for Water Radiolysis”

1. A. Gulea, D. Poirier, J. Roy, V. Stavila, V. Tapcov, *Moldovan Patent MD-2786* (**2005**).

 “Inhibitors of Human Myeloid Leukemia Based on Heteronuclear Coordination Compounds of Cobalt(III) and Bismuth(III)”

1. A. Gulea, V. Stavila, V. Tapcov, I. Bulimestru, *Moldovan Patent MD-2479* (**2004**).

“Dodecahydrate of (diethylene-triamine-penta-acetato)bismuthate(III) of Hexaaminocobalt(III) as a Dielectric Material”

1. A. Gulea, V. Stavila, V. Tapcov, A. Paraschivescu, A. Cecal, *Moldovan Patent MD-2450* (**2004**).

“Catalyst for Radiolytic Decomposition of Water for Hydrogen Production”

1. A. Gulea, V. Stavila, V. Tapcov, *Moldovan Patent MD-2240* (**2003**).

“Tris(thiosemicarbazide)cobalt(III) bis(nitrilotriacetato)bismuthate(III) Nonahydrate as a Dielectric Material”

1. A. Gulea, V. Stavila, V. Tapcov, *Moldovan Patent MD-2146* (**2003**).

 “Dielectric Materials Based on Heteronuclear Coordination Complexes of Cobalt(III) and Bismuth(III)”

1. A. Gulea, V. Stavila, I. Bulimestru, J.-P. Wignacourt, V. Tapcov. *Moldovan Patent MD-1559* (**2000**).

“Process for Obtaining Bismuth Cuprate”

**Book Chapters**

1. V. Stavila, L.E. Klebanoff, J.J. Vajo, P. Chen, “Development of On-Board Reversible Complex Metal Hydrides for Hydrogen Storage” in *Hydrogen Storage Technology: Materials and Applications, Ed. L.E. Klebanoff,* Taylor and Francis, Boca Raton,**2012***, pages 133-213.*
2. V. Stavila, L.E. Klebanoff, *“Hydrogen – Metal hydride storage” in “Hydrogen: Data, Facts and Figures”, Eds. D. Stolten and R.C. Samsun*, Wiley-VCH, Dortmund, **2015**, *pages 79–93.*