

## 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. with Honors / Chemistry**

State University of Moldova, Chisinau, Moldova, 1996

### PROFESSIONAL EXPERIENCE

- **2008 – present**

*Research Scientist*

Principal investigator on an U.S. Department of Energy sponsored project devoted to synthesis of complex metal hydride 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

Management of the X-Ray diffraction facility at Sandia-California site

Synthesis and characterization of nanomaterials for energy harvesting and storage

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

- **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

## 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.
- 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,  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{11}\text{B}$ ,  $^{27}\text{Al}$  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.

## 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

## AFFILIATIONS

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

## PROFESSIONAL SERVICE

Proposal Reviewer: *DOE EERE, ARPA-E, NSF, CRDF, INTAS, SCOPES*  
Editorial Board Member: *Materials (MDPI)*  
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*

## PUBLICATIONS

Published more than 140 articles in peer-reviewed journals, 2 book chapters and 15 US and international patents.

## Publication list (as of September 2019)

### Peer-Reviewed Journal Articles:

1. 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"
2. 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"
3. 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"
4. 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"
5. 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 MgB<sub>2</sub> to Mg(BH<sub>4</sub>)<sub>2</sub> upon Mechanical Milling with THF, MgH<sub>2</sub>, and/or Mg"
6. 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"
7. 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 NaAlH<sub>4</sub>"
8. 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"
9. 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"
10. Schneemann, A.; White, J. L.; Kang, S.Y.; 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"
11. 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"
12. 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 Cu<sub>3</sub>BTC<sub>2</sub> Thin Films Before and After Reaction with TCNQ"
  13. 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"
  14. 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 LiCB<sub>11</sub>H<sub>12</sub> and NaCB<sub>11</sub>H<sub>12</sub>"
  15. 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 H<sub>2</sub> Desorption Rate of NaAlH<sub>4</sub> Confined in Nitrogen-Doped Nanoporous Carbon Frameworks"
  16. 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"
  17. 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: Rb<sub>2</sub>B<sub>10</sub>H<sub>10</sub>"
  18. 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, B<sub>10</sub>H<sub>10</sub><sup>(2-)</sup> and B<sub>12</sub>H<sub>12</sub><sup>(2-)</sup>, composites."
  19. 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"
  20. 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 TiCl<sub>3</sub> and TiF<sub>3</sub> with hydrogen"
  21. 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"
  22. 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"
  23. 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"
24. 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  $(\text{NH}_4)_2\text{B}_{12}\text{H}_{12}$ "
25. 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"
26. 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"
27. 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"
28. 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"
29. 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"
30. 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  $\text{B}_{12}\text{F}_{12}^{2-}$ ,  $\text{B}_{12}\text{Cl}_{12}^{2-}$ , and  $\text{B}_{12}\text{H}_{12}^{2-}$  to  $\text{Na}^+$  in the Solid State: Crystal Structures and Thermal Behavior of  $\text{Na}_2(\text{B}_{12}\text{F}_{12})$ ,  $\text{Na}_2(\text{H}_2\text{O})_4(\text{B}_{12}\text{F}_{12})$ ,  $\text{Na}_2(\text{B}_{12}\text{Cl}_{12})$ , and  $\text{Na}_2(\text{H}_2\text{O})_6(\text{B}_{12}\text{Cl}_{12})$ "
31. 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"
32. Dolgoplova, 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"
33. 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  $\text{MCB}_9\text{H}_{10}$  and  $\text{M}_2\text{B}_{10}\text{H}_{10}$  ( $\text{M} = \text{Li}, \text{Na}$ ) via Nuclear Magnetic Resonance and Quasielastic Neutron Scattering Studies"
34. 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”
35. 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 MgB<sub>2</sub> initial hydrogenation via a combined experimental-theoretical study”
36. 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”
37. 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”
38. M.D Allendorf, V. Stavila, *Nature Materials*, **2016**, *15*, 255-257.
- “Nanoporous films: From conventional to conformal”
39. 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”
40. 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(BH<sub>4</sub>)<sub>2</sub> polymorphs probed with neutron vibrational spectroscopy and first-principles calculations”
41. 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”
42. 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”
43. 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”
44. 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”
45. 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”
46. 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: NaCB<sub>9</sub>H<sub>10</sub>”
47. 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”
48. 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)”
49. 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 TiS<sub>2</sub> and LiBH<sub>4</sub> in bulk-type all-solid-state lithium batteries”
50. M.D. Allendorf, V. Stavila, *CrystEngComm*, **2015**, *17*, 229–246.
- “Crystal engineering, structure-function relationships, and the future of metal-organic frameworks”
51. 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.
- “Stable interface formation between TiS<sub>2</sub> and LiBH<sub>4</sub> in bulk-type all-solid-state lithium batteries”
52. H. Wu, W.S. Tang, W. Zhou, V. Stavila, J.J. Rush, T.J. Udovic, *CrystEngComm*, **2015**, *17*, 3533-3540.
- “The structure of monoclinic Na<sub>2</sub>B<sub>10</sub>H<sub>10</sub>: a combined diffraction, spectroscopy, and theoretical approach”
53. 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”
54. 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”
55. K.R. Reyes-Gil, Z.D. Stephens, V. Stavila, D.B. Robinson, *ACS Applied Materials & Interfaces*, **2015**, *7*, 2202-2213.
- “Composite WO<sub>3</sub>/TiO<sub>2</sub> nanostructures with high electrochromic activity”
56. 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 LiCB<sub>11</sub>H<sub>12</sub> and NaCB<sub>11</sub>H<sub>12</sub>: <sup>1</sup>H, <sup>7</sup>Li, and <sup>23</sup>Na NMR Studies”
57. 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”
58. 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 Li<sub>2</sub>B<sub>10</sub>H<sub>10</sub>”
59. W.S. Tang, T.J. Udovic, V. Stavila, *Journal of Alloys and Compounds*, **2015**, *645*, S200-S204. “Altering the structural properties of A<sub>2</sub>B<sub>12</sub>H<sub>12</sub> compounds via cation and anion modifications”
60. 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*”
61. 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”
62. 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”
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## Patents

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“Dodecahydrate of (diethylene-triamine-penta-acetato)bismuthate(III) of Hexaaminocobalt(III) as a Dielectric Material”
12. A. Gulea, V. Stavila, V. Tapcov, A. Paraschivescu, A. Cecal, *Moldovan Patent MD-2450 (2004)*.  
“Catalyst for Radiolytic Decomposition of Water for Hydrogen Production”
13. A. Gulea, V. Stavila, V. Tapcov, *Moldovan Patent MD-2240 (2003)*.  
“Tris(thiosemicarbazide)cobalt(III) bis(nitritotriacetato)bismuthate(III) Nonahydrate as a Dielectric Material”
14. A. Gulea, V. Stavila, V. Tapcov, *Moldovan Patent MD-2146 (2003)*.  
“Dielectric Materials Based on Heteronuclear Coordination Complexes of Cobalt(III) and Bismuth(III)”
15. 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.

## Selected Conference Presentations

1. "Understanding Hydrogen Desorption Pathways in Nanoscale Metal Hydrides", Stavila, V. Gordon Research Conference on Hydrogen-Metal Systems, Spain, **2019**.
2. "Ion dynamics of hydride-based solid electrolytes for battery applications", Stavila, V.; Udovic, T. LIMBAT Conference, Lillestrøm, Norway, **2018**.
3. "Computational studies of kinetic mechanisms governing hydrogen interactions with complex hydrides", Wood, B.; Ray, K.; Heo, T. W.; Kang, S.; Lee, J.; Baker, A.; Rowberg, A.; Ogitsu, T.; Shi, R. P.; Klebanoff, L.; Stavila, V.; Allendorf, M. *255<sup>th</sup> American Chemical Society National Meeting*, New Orleans, LA, **2018**.
4. "Rapid hydrogen-deuterium exchange in metal-organic frameworks", Stavila, V.; Wang, T.; Cowgill, D.; Allendorf, M. *255<sup>th</sup> American Chemical Society National Meeting*, New Orleans, LA, **2018**.
5. "Multifunctional metal-organic framework catalysts for hydrogen activation", V. Stavila, R. Bhakta, T. Alam, E.H. Majzoub, M.D. Allendorf. *255<sup>th</sup> American Chemical Society National Meeting*, New Orleans, LA, **2018**.
6. "Catalytically functionalized nanoporous frameworks and carbons for chemical energy storage", Allendorf, M.; Brown, J.; White, J.; Stavila, V.; Heo, T. W.; Wood, B.; Klebanoff, L. *254<sup>th</sup> American Chemical Society National Meeting*, Washington DC, **2017**.
7. "Anion dynamical behaviors and their possible relationship to superionic conductivities in hydro-closo-borate salts of lithium and sodium", Dimitrievska, M.; Tang, W. S.; Kweon, K.; Wood, B.; Shea, P.; Varley, J.; Stavila, V.; Skripov, A.; Yoshida, K.; Orimo, S.; Udovic, T. *254<sup>th</sup> American Chemical Society National Meeting*, Washington DC, **2017**.
8. "Bioinspired MOF design for lignin catalysis: Role of co-factor on enzymatic lignolysis", Ramakrishnan, P.; Stavila, V.; Simmons, B.; Allendorf, M.; Sale, K. *251<sup>st</sup> American Chemical Society National Meeting*, San Diego, CA, **2016**.
9. "MOF-based catalysts for lignin degradation", V. Stavila, R. Bhakta, T. Alam, E.H. Majzoub, M.D. Allendorf. *245<sup>th</sup> American Chemical Society National Meeting*, New Orleans, LA, **2013**.
10. "Metal-organic frameworks as nanoreactors for reversible de/rehydrogenation reactions", Allendorf, M. D.; Davis, R. W.; Ramakrishnan, P.; Sale, K. L.; Stavila, V. *248<sup>th</sup> American Chemical Society National Meeting*, San Francisco, CA, **2014**.
11. "Integrating MOFs with MEMS devices for sensing", M.D. Allendorf, J.M. Denning, J.A. Greathouse, A.L. Robinson, T.R. Zeitler, V. Stavila. *245<sup>th</sup> American Chemical Society National Meeting*, New Orleans, LA, **2013**.

12. "Metal-Organic Frameworks as Scaffolds for Reversible Complex Metal Hydrides", V. Stavila, R. Bhakta, T. Alam, E.H. Majzoub, M.D. Allendorf. *244<sup>th</sup> American Chemical Society National Meeting*, Philadelphia, PA, **2012**.
13. "Fabrication of MOF Thin Films for Chemical Sensing", V. Stavila, J. Volponi, K. Leung, A.L. Robinson, I. Ellern, P.J. Hesketh, M.D. Allendorf. *243<sup>rd</sup> American Chemical Society National Meeting*, San Diego, CA, USA, **2012**.
14. "Improvement of Hydrogen Storage Properties of Complex Metal Hydrides Through Hydridic-Protic Interactions", V. Stavila. *19<sup>th</sup> World Hydrogen Energy Conference*, Toronto, Canada, **2012**.
15. "Metal-organic frameworks for greenhouse gas detection", Allendorf, M. D.; Zeitler, T. R.; Robinson, A. L.; Stavila, V. *242<sup>nd</sup> American Chemical Society National Meeting*, Denver, CO, USA, **2011**.
16. "Hydridic-protic interactions in complex metal hydrides", V. Stavila, W. Luo, M. E. Majzoub, R. Behrens, L. Klebanoff. *242<sup>nd</sup> American Chemical Society National Meeting*, Denver, CO, USA, **2011**.
17. "Complex metal hydrides for hydrogen storage applications", V. Stavila, (Invited talk). *Energy Storage and Intermittent Renewable Energy*, Santa Clara, CA, USA, **2010**.
18. "Hydrogen storage in alkali and alkaline earth borohydrides: Probing the role of intermediate species", V. Stavila, R.J. Newhouse, S.-J. Hwang, M. Ulutagay-Kartin, J.-H. Her, T.J. Udovic (Invited talk). *239<sup>th</sup> American Chemical Society National Meeting*, San Francisco, CA, USA, **2010**.
19. "Catalyzed magnesium borohydride: Hydrogen desorption and rehydrogenation", R. Newhouse, V. Stavila, S. Hwang, J. Zhang. *239<sup>th</sup> American Chemical Society National Meeting*, San Francisco, CA, USA, **2010**.
20. "Factors Affecting Hydrogen Release from Metal Borohydrides" V. Stavila, E.H. Majzoub, S.-J. Hwang, R.J. Newhouse, M. Ulutagay-Kartin, W. Luo, J.G. Cordaro, T.J. Udovic. Oral Presentation. *Materials Challenges in Alternative and Renewable Energy*, Cocoa Beach, Florida, USA, **2010**.
21. "Hydrogen multinuclear high resolution NMR Studies of dodecaborate intermediate of borohydride-based hydrogen storage systems", S.-J. Hwang, C. Ahn, J. W. Reiter, J. A. Zan, V. Stavila, J. J. Vajo. Oral Presentation. *Materials Challenges in Alternative and Renewable Energy*, Cocoa Beach, Florida, USA, **2010**.
22. "Combining first principles and thermodynamic calculations to predict evolution of impurity gases from metal hydrides", M. Allendorf, V. Stavila, K.C. Kim, D.S. Sholl (Invited talk). *239<sup>th</sup> American Chemical Society National Meeting*, San Francisco, CA, USA, **2010**.
23. "Alkali and alkaline-earth dodecahydro-closo-dodecaborates and their relevance to hydrogen storage" V. Stavila, J.-H. Her, M. Ulutagay-Kartin, W. Zhou, S.-J. Hwang, Ch. Kim, T.J. Udovic. Oral Presentation. *238<sup>th</sup> American Chemical Society National Meeting*, Washington, DC, USA, **2009**.
24. "Crystal structures of  $M_nB_{12}H_{12}$  ( $n=1,2$ ) compounds – possible intermediate species in the decomposition of  $M(BH_4)_n$ " J.-H. Her, V. Stavila, M. Yousufuddin, W. Zhou, S.S. Jalilati, E. Rönnebro, T.J. Udovic. Oral Presentation, accepted. *American Crystallographic Association Meeting*, Toronto, Canada, **2009**.
25. "Discovery and development of metal borohydrides: Calcium borohydride, new bialkali- and transition metal borohydrides". E. Rönnebro, E. Majzoub, L. Seballos, R. Newhouse, R.C. Bowman, Jr., Sonjong Hwang, C. Kim, G. Severa, C. Jensen, M. Kartin, V. Stavila. Oral Presentation. *International Symposium on Metal-Hydrogen Systems*, Reykjavik, Iceland, **2008**.
26. "Spin-state variable, iron-based, enzyme-responsive MRI contrast agents: Evaluation of two molecule candidates employing distinct auto-immolable architectures". N. Kuznik, V. Stavila, M.

- Allali, Y. Stortz, P. Maurin, J. Hasserodt. Oral Presentation. *226<sup>th</sup> ACS National Meeting*, Philadelphia, PA, USA, **2008**.
27. "New materials based on bismuth-lanthanide coordination compounds". A. Gulea, V. Stavila, N. Popa, I. Bulimestru, L. Culiuc, A. Siminel, O. Kulikova, K.H. Whitmire. Poster Presentation. *38<sup>th</sup> International Conference on Coordination Chemistry*, Jerusalem, Israel, **2008**.
28. "Solvothermal synthesis of lead sulfide nanostructures from single-source precursors". T. Mandal, V. Stavila, K.H. Whitmire. Oral Presentation. *225<sup>th</sup> ACS National Meeting*, New Orleans, LA, USA, **2008**.
29. "Arylation reactions of bismuth carboxylates". K.H. Whitmire, J.H. Thurston, V. Stavila, D. Prieto-Centurion. Oral Presentation. *223<sup>rd</sup> ACS National Meeting*, Chicago, IL, USA, **2007**.
30. "New bismuth(III)-lanthanide(III) coordination compounds as molecular precursors for heterometallic oxide materials". V. Stavila, K.H. Whitmire, N. Popa, I. Bulimestru, A. Gulea. Poster Presentation. *XXIII International Chugaev Conference on Coordination Chemistry*. Odessa, Ukraine. **2007**.
31. "Spin-state variable, iron-based, enzyme-responsive MRI contrast agents: Evaluation of a first molecule candidate using auto-immolable spacer technology". V. Stavila, L. Canaple, O. Beuf, M. Allali, Y. Stortz, P. Maurin, J. Samarut, M. Janier, J. Hasserodt. Poster Presentation. *13<sup>th</sup> International Conference on Biological Inorganic Chemistry*. Vienna, Austria, **2007**.
32. "Coordination compounds based on bismuth salicylates". I. Bulimestru, V. Stavila, K. H. Whitmire, A. Gulea. Poster Presentation. *29<sup>th</sup> Romanian Chemical Conference*, Calimanesti, Romania, **2006**.
33. "Structure and thermal behavior of new Cr(III)-Bi(III) complexes". V. Stavila, I. Bulimestru, A. Gulea, K. Whitmire. *29<sup>th</sup> Romanian Chemical Conference*, Calimanesti, Romania, **2006**.
34. "Crystal structures of some 3d elements–Bi(III) heterobimetallic complexes and their antileukemia activity". A. Gulea, D. Poirier, J. Roy, V. Stavila, I. Bulimestru. Poster Presentation. *11<sup>th</sup> International Conference on Crystallization of the BioMacromolecules (ICCBM)*, Quebec, Canada, **2006**.
35. "Heteronuclear coordination compounds of bismuth(III) and some 3d metals as catalysts for producing non-polluting fuel". I. Bulimestru, V. Stavila, A. Cecal, A. Paraschivescu, V. Tsapcov, A. Gulea. Poster Presentation. *3<sup>rd</sup> International Conference "Ecological Chemistry"*, Chisinau, Moldova, **2005**.
36. "Crystal and molecular structures of  $[\text{Bi}_2(\text{EDTA})_2](\text{Hphen})_2 \cdot 8\text{H}_2\text{O}$  and  $[\text{VO}(\text{NTA})(\text{H}_2\text{O})](\text{Hphen}) \cdot \text{H}_2\text{O}$ ". P. Petrenco, Yu. Simonov, M. Gdaniec, A. Gulea, V. Stavila. Poster Presentation. *22<sup>nd</sup> Chugaev International Conference on Coordination Chemistry*, Chisinau, Moldova, **2005**.
37. "From bismuth complexonates to bismuth perovskites". A. Gulea, P. Petrenco, I. Bulimestru, V. Stavila, S. Shova, M. Gdaniec, Yu. Simonov. Poster Presentation. *2<sup>nd</sup> International Conference on Materials Science and Condensed Matter Physics*, Chisinau, Moldova, **2004**.
38. "Two novel 3D Nd(III)-Bi(III) aminopolycarboxylate coordination polymers". V. Stavila, A. Gulea, N. Popa, S. Shova, A. Merbach, Y. Simonov, J. Lipkowski. Poster Presentation. *5<sup>th</sup> International Conference on f-Elements*, Geneva, Switzerland, **2003**.
39. "An unexpected influence of the nature of the amine on the crystal structure of some Co-Bi heterometallic complexes". V. Stavila, A. Gulea, S. Shova, Yu. Simonov, J. Lipkowski, P. Petrenco. Poster Presentation. *21<sup>st</sup> Chugaev International Conference on Coordination Chemistry*. Kiev, Ukraine, **2003**.