

First Name: Vitalie
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Job Title: Senior Member of Technical Staff
Department Name: Hydrogen and Combustion Technologies

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Vitalie Stavila
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SHORT BIO:
 (250 words or less)

Vitalie Stavila received his PhD. in chemistry from Moldova State University (2002) working with Prof. A. Gulea in inorganic chemistry. He had postdoctoral stays at Ecole Normale Supérieure de Lyon, France, working with Prof. Jens Hasserodt on spin-active contrast agents for magnetic resonance imaging and at Rice University in Houston, TX working with Prof. Ken Whitmire to develop organometallic precursors for nanostructured metal oxides and chalcogenides. Dr. Stavila joined Sandia in 2008 to develop materials and nanostructures for energy harvesting and storage. He served as a PI in the DOE Metal Hydride Center of Excellence developing reversible metal hydrides for hydrogen storage applications. He has also provided new insights into porous materials preparation and functionalization and their use as nanoscaffolds in catalysis and chemical sensing. In his current research Dr. Stavila uses various X-ray scattering and diffraction techniques to solve fundamental and applied materials science problems related to bulk and nanostructured metal hydrides, oxides, chalcogenides, organometallic compounds, and metal-organic frameworks. Dr. Stavila has published over 80 peer-reviewed research articles, 2 book chapters, and 7 patents.

RESEARCH INTERESTS

Dr. Vitalie Stavila's research is focused on addressing key materials science challenges related to energy generation and storage. His main research interests are in the area of functional materials (including metal hydrides, oxides, chalcogenides, organometallic compounds, metal-organic frameworks) where he uses a range of synthetic, spectroscopic, diffraction and knowledge mining techniques to probe the processing-structure-property relations in materials. His current projects focus on the development of novel multifunctional materials and nanostructures for energy storage and nanoscale fabrication. He is also involved in the development of new organometallic compounds and metal-organic frameworks that can act as active materials in scintillators, sensors, photovoltaic devices and gas storage. A central theme in Dr. Stavila's research is the rational design of new materials by changing the chemical composition, the arrangement of the atoms or molecules in crystalline or amorphous configurations, and the size, shape, and orientation of nanoparticles, crystals or other nano- or macroscopic units. In his work Dr. Stavila employs a variety of X-ray diffraction and scattering techniques, including powder X-ray diffraction and microdiffraction, Rietveld refinement and single-crystal X-ray crystallography.

EDUCATION

State University of Moldova, Chisinau, Moldova

Ph.D. / Chemistry, 2002

Thesis title: "Synthesis of bismuth-transition metal heterobimetallic complexes as molecular precursors for mixed oxide systems"

AWARDS, HONORS AND MEMBERSHIPS

- U.S. Department of Energy Hydrogen Program "Special Recognition Award" for the achievements of the Metal Hydride Center of Excellence team, 2010
- Welch Fellowship, Department of Chemistry, Rice University, 2007
- Civilian Research and Development Foundation Research Award, 2006
- NSF-NATO Postdoctoral Fellowship Award, 2005
- National Award for Young Scientists in the field of Science and Technology, Moldova, 2004
- Young Scientist of the Year Research Award, Moldova, 2003
- European Rare Earth and Actinide Society Award, Geneva, Switzerland, 2003

SELECTED PUBLICATIONS

Journal articles

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"
2. N. Verdal, J.-H. Her, V. Stavila, A.V. Soloninina, 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 $\text{Li}_2\text{B}_{12}\text{H}_{12}$ and $\text{Na}_2\text{B}_{12}\text{H}_{12}$ "
3. T.J. Udovic, M. Matsuo, A. Unemoto, N. Verdal, V. Stavila, A.V. Skripov, J.J. Rush, H. Takamure, S. Orimo, *Chemical Communications*, **2014**, DOI:10.1039/C3CC49805K.
"Sodium superionic conduction in $\text{Na}_2\text{B}_{12}\text{H}_{12}$ "
4. 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"
5. V. Stavila, R.K. Bhakta, T.M. Alam, E.H. Majzoub, M.D. Allendorf, *ACS Nano*, **2012**, 6, 9807-9817.
"Reversible Hydrogen Storage by NaAlH_4 Confined within a Titanium-Functionalized MOF-74(Mg) Nanoreactor"
6. G. Cheng, P. Varanasi, R. Arora, C. Scullin, V. Stavila, B.A. Simmons, S. Singh, *J. Phys. Chem. B*, **2012**, 116, 10049-10054.
"Impact of ionic liquid pretreatment conditions on cellulose crystalline structure using 1-ethyl-3-methylimidazolium acetate"
7. 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 Thin Film Growth: Systematic Investigation of HKUST-1 Deposition on QCM Electrodes"
8. 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"
9. 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"
10. 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"

11. 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-*clos*-dodecaborate: Synthesis, Structure and Relevance to Hydrogen Storage”
12. R. Newhouse, V. Stavila, S. Hwang, J. Zhang, *Journal of Physical Chemistry, C* **2010**, *114*, 5224–5232.
“Reversibility and Improved Hydrogen Release of Magnesium Borohydride”
13. 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”
14. 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”
15. V. Stavila, I. Rusakova, K.H. Whitmire, *Chemistry of Materials*, **2009**, *21*, 5456–5465.
“Synthesis of Bi_2S_3 Nanostructures from Bismuth(III) Thiourea and Thiosemicarbazide Complexes”
16. 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”
17. V. Stavila, E. Dikarev, *Journal of Organometallic Chemistry*, **2009**, *694*, 2956–2964.
“Phenyl Bismuth Beta-Diketonate Complexes: Synthesis and Structural Characterization”
18. V. Stavila, J.H. Thurston, K.H. Whitmire, *Inorganic Chemistry*, **2009**, *48*, 6945–6951.
“Selective Arylation Reactions of Bismuth-Transition Metal Salicylate Complexes”
19. 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-Immobilable Pendant Arm by Iron Coordination”
20. V. Stavila, J.C. Fettinger, K.H. Whitmire, *Organometallics*, **2007**, *26*, 3321–3328.
“Synthesis and characterization of new phenylbis(salicylato)-bismuth(III) complexes”
21. 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”
22. 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 the EDTA ligand”

Book Chapter

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.