

## PUBLICATIONS AND PRESENTATIONS

M. D. Allendorf  
1985 – 2017

### Journal articles

1. He, Y, CD Spataru, F Léonard, RE Jones, ME Foster, M Allendorf, AA Talin. (2017). Two-Dimensional Metal-Organic Frameworks with High Thermoelectric Efficiency Through Metal Ion Selection, *Physical Chemistry Chemical Physics*, accepted.
2. A. M. Ullman, J. W. Brown, M. E. Foster, F. Léonard, K. Leong, V. Stavila, M. D. Allendorf “Transforming MOFs for Energy Applications Using the Guest@ MOF Concept,” *Inorganic Chemistry* **55** (15), 7233 (2016).
3. 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, and A. A. Talin “Thin Film Thermoelectric Metal-Organic Framework with High Seebeck Coefficient and Low Thermal Conductivity,” *Advanced Materials*, **27**, 3453-3459 (2015).
4. M. D. Allendorf, M. E. Foster, F. Léonard, V. Stavila, P. L. Feng, F. P. Doty, K. Leong, E.Y. Ma, S. R. Johnston, A. A. Talin “Guest-Induced Emergent Properties in Metal-Organic Frameworks,” *J. Phys. Chem. Lett.*, **6** (7), pp 1182-1195 (2015).
5. D. J. Spira, M. D. Allendorf, E. I. Solomon “Selective Chemical and Physical Perturbations for the Different Copper Sites in the Multicopper Oxidase, Rhus Laccase,” *Inorg. Chim. Acta* **79** (1983), 130, DOI: 10.1016/S0020-1693(00)95162.4.
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11. P. K. Ross, M. D. Allendorf, E. I. Solomon “Detailed Spectral Studies of Copper Acetate: Excited-State Interactions in Copper Dimers,” *J. Am. Chem. Soc.* **111** (1989), 4009, DOI: 10.1021/ja00193a038.
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3. J. J. Perry IV, C. A. Bauer, M. D. Allendorf "Luminescent Metal-Organic Frameworks," *Applications of Metal-Organic Frameworks*, D. Farrusseng, ed., Wiley-VCH, Weinheim, published July 2011.

### **News items, professional society articles, editorials**

1. A. C. Khandkar, K. Spear, M. Allendorf "High Temperature Materials--Past, Present, and Future" *Interface*, **5**, 25, 1996.

2. M. D. Allendorf "From Bunsen to ULSI: 150 Years of Growth in Chemical Vapor Deposition Technology," *Interface* **7** (1998), No.1, 36.
3. M. D. Allendorf "EUROCVI-12" *Adv. Mat./Chem. Vapor Dep.*, **9**, 6, 2000, Essay reviewing the 12<sup>th</sup> EUROCVI meeting in Barcelona, Spain.
4. A. H. McDaniel, M. D. Allendorf, R. J. McCurdy "Devices for Monitoring Process Chemistry in Coated Float Glass," *Glass Researcher*, **10**, 1, 12, 2000.
5. M. D. Allendorf "Research Needs for Coatings on Glass: Summary of the U.S. Department Of Energy Roadmapping Workshop," *Thin Solid Films* **392**, 2, 2001, 155-163, DOI: 10.1016/S0040-6090(01)01021-5.
6. M. D. Allendorf "On-Line Deposition of Oxides on Flat Glass," *Interface*, **10**, 2, 2001.
7. A. M. B. van Mol, G. R. Alcott, M. D. Allendorf "Understanding tin oxide precursor chemistry and its link to coating properties," *Ceramic Bulletin*, **84**, 37, 2005.
8. M. D. Allendorf "The Essential and the Nonessential," 'From the President' column *Interface*, **15**, 2, 2006, 7.
9. M. D. Allendorf "Doing Science by the Numbers," 'From the President' column *Interface*, **15**, 3, 2006, 7.
10. M. D. Allendorf "Multiple Realities," 'From the President' column *Interface*, **15**, 4, 2006, 7.
11. M. D. Allendorf "New Directions, New Ideas," 'From the President' column *Interface*, **16**, 1, 2007, 7.
12. M. D. Allendorf, F. P. Doty, P. L. Feng "Designer Colors for Radiation Detection" in *SPIE Newsroom* (2012): 3p. Published electronically 18 September 2012.  
DOI:10.1117/2.1201209.004465.

### **Invited presentations**

1. M. D. Allendorf "Thermochemistry and Kinetics of Gas-Phase Reactions in the CVD of Ceramic Materials," presented at *Stanford University*, February 7, 1996.
2. M. D. Allendorf "Kinetics of Gas-Phase and Surface Reactions in the CVD of Ceramic Materials," presented at the *National Institute of Standards and Technology*, Washington, DC, April 10, 1996.
3. M. D. Allendorf "Thermochemistry and Kinetics of Gas-Phase Reactions in the Chemical Vapor Deposition of Ceramic Materials" presented at *NASA Ames Research Center*, March 13, 1997.
4. M. D. Allendorf "Gas-Phase Thermochemistry and Kinetics Relevant to the CVD of Ceramic Materials: New Data for Process Models," presented at *Laboratoire de Thermodynamique et Physicochimie Metallurgiques, Centre National de Recherche Scientifique (CNRS)*, Grenoble, France, September, 1997.
5. M. D. Allendorf "Gas-Phase Thermochemistry and Kinetics Relevant to the CVD of Ceramic Materials: New Data for Process Models," presented at *Institut de Science et de Génie des Matériaux et Procédés, CNRS*, Perpignan, France, September, 1997.
6. M. D. Allendorf "Gas-Phase Thermochemistry and Kinetics Relevant to the CVD of Ceramic Coatings: New Data for Process Models," presented at *Int. Conf. Met. Coatings Thin Films*, San Diego, April, 1998.
7. M. D. Allendorf, S. Ferko, A. McDaniel, C. F. Melius "Thermochemistry and Kinetics for CVD Modeling: Good News and Bad News," presented at *Gordon Conf/HTChem.*, July 21, 1998.
8. M. D. Allendorf, C. F. Melius, A. H. McDaniel "Thermochemistry and Kinetics of Gas-Phase Reactions Relevant to the CVD of Coatings: New Data for Process Models," presented in *Properties and Processing of Vapor Deposited Coatings, Fall Meeting of the Materials Research Society*, November 31 – December 4, 1998.
9. M. D. Allendorf "High-Temperature Thermochemistry and Kinetics for Modeling CVD: A Shotgun Marriage Between Experiments and Theory," presented in the *Dept. of Materials Science*, Penn State University, December 3, 1998.
10. C. F. Melius, M. D. Allendorf "The Determination of Thermochemical Data for CVD Using *Ab Initio* Quantum Chemistry Methods," *CALPHAD XXVIII*, Grenoble, France, May 2-7, 1999.

11. M. D. Allendorf, A. H. McDaniel, C. F. Melius, F. Teyssandier, C. Raffy “Thermochemistry and Kinetics of Chemical Reactions Relevant to the CVD of Ceramics and Hard Coatings: An Integrated Experimental and Modeling Approach,” *Fall Meeting of the AIChE*, Dallas, TX, November 1, 1999.
12. M. D. Allendorf “Thermochemistry and Kinetics of Chemical Reactions Relevant to CVD: New data for Process Models,” *Corning/Sullivan Park Research Center*, Corning, NY, December 8, 1999.
13. A. H. McDaniel, M. D. Allendorf “Advanced Microanalytical Devices for On-line Process Monitoring of CVD Reactors in a Float Glass Facility,” *IFPAC Conference*, Las Vegas, January 27, 2000.
14. M. D. Allendorf, K. E. Spear “Thermodynamic Analysis of Silica Refractory Corrosion in Glass-Melting Furnaces,” *Glass and Optical Materials Division Meeting of the American Ceramic Society*, Corning, NY, October 1-4, 2000.
15. M. D. Allendorf, “Research Needs for Coatings on Glass: Summary of the U.S. Department Of Energy Roadmapping Workshop,” keynote lecture, *Third Int. Conf. Coatings on Glass*, Maastricht, The Netherlands, October 29 - November 2, 2000.
16. M. D. Allendorf “Gas-Phase Chemistry in the On-Line Deposition of Coatings on Float Glass,” *Int. Conf. Metallurgical Coatings and Thin Films*, San Diego, April 30 - May 4, 2001.
17. M. D. Allendorf “Thermodynamic and Transport Modeling of Refractory Corrosion in Glass-Melting Furnaces,” *PPG Glass Technology Center*, Cheswick, PA, May 16, 2001.
18. M. D. Allendorf “Using Theory and Experiment to Understand the Chemistry of Chemical Vapor Deposition,” *PPG Glass Technology Center*, Cheswick, PA, May 15, 2001.
19. K. E. Spear, M. D. Allendorf “Thermodynamic Calculations Involving Reactions between Glass and Refractories,” *American Ceramic Soc. 104<sup>th</sup> Annual Meeting*, St. Louis, MO, April 28 – May 1, 2002.
20. M. D. Allendorf, “Soup to Nuts Modeling of High-Temperature Chemistry in Industrial Processes: Quantum Chemistry to Experimental Validation,” *Dept. of Chemistry, Univ. Strathclyde*, Glasgow, Scotland, December 6, 2002.
21. M. D. Allendorf “Modeling High-Temperature Chemistry in Industrial Processes: Quantum Chemistry to Experimental Validation,” *Dept. of Chem. Eng., Univ. Louisville*, February 26, 2003.
22. M. Allendorf, R. Nilson, B. Bugeat, A. Gupta, O. Marin, K. E. Spear “Analytical Models For High-Temperature Corrosion Of Silica Refractories In Glass-Melting Furnaces,” *7th Int. Conf. Adv. Fusion Processing of Glass*, Rochester, NY, July 27-30, 2003.
23. M. D. Allendorf “ $\mu$ ChemLab<sup>TM</sup>: A Hand-Portable Microanalytical Instrument for BioAnalysis,” Sandia National Laboratories, Center 1700, May 19, 2004.
24. T. A. M. B. van Mol, Y. Chae, A. H. McDaniel, M. D. Allendorf “Chemical vapour deposition of tin oxide: fundamentals and applications,” keynote lecture, *5<sup>th</sup> Int. Conf. Coatings on Glass*, Saarbruecken, Germany, July 4–8, 2004.
25. M. D. Allendorf “Quantum Chemistry, the Web, and You: Using Computers to Generate a Really Useful Thermodynamic Database,” *CHEMKIN workshop, Int. Comb. Symp.* Chicago, IL, July 25, 2004.
26. M. D. Allendorf “Quantum Chemistry for the Masses: Development of an On-Line Thermochemical Database (with illustrations from the MOCVD of 4th-Row Main Group Oxides),” *Ruhr Universität Bochum, Inorganic and Physical seminar series*, December 10, 2004.
27. M. D. Allendorf “Ab Initio Predictions of Thermochemistry for Gas-Phase Tin, Indium, and Antimony Compounds Relevant to CVD Coatings on Glass,” *TNO TPD*, Eindhoven, The Netherlands, December, 2004.
28. M. D. Allendorf “ $\mu$ ChemLab<sup>TM</sup>: A Hand-Portable Microanalytical Instrument for BioAnalysis (and other tales of why small is big...),” *Georgia Tech*, March 10, 2005.
29. R. A. Fischer, S. Hermes, F. Schröder, C. Wöll, M. Allendorf, “Metal@MOFs: perspectives of metal organic open frameworks as novel host matrices for imbedding functional nanoparticles,” invited lecture, *SAMIC Trends in Nanoscience conference*, Bressanone, Italy, December 4-7, 2005.

30. M. D. Allendorf “Reflections on a Career at a National Laboratory,” invited lecture, *University of California, Davis Laboratory Management Institute 2005-2006 Postdoctoral Program*, June 6, 2006.
31. T. M. Besmann, N. S. Kulkarni, K. E. Spear, M. D. Allendorf “Thermochemical Modeling of High Temperature Behavior of Chemically Complex Oxide Glass Solutions,” *Int. Conference on Glass*, Sunderland, United Kingdom, September, 2006.
32. M. D. Allendorf “Metal Organic Frameworks: Nanoporous Materials for Sensing, Separations, and More,” Dept. of Chemical Engineering, University of Colorado, Boulder, CO, October 12, 2006.
33. N. Siegel, J. E. Miller, M. D. Allendorf, R. J. Diver “Hydrogen Production Research in the United States,” keynote lecture, *Fusion 2007 symposium*, Nagata, Japan, January 10-12, 2007.
34. J. E. Miller, M. D. Allendorf, R. B. Diver, L. R. Evans, N. P. Siegel, J. N. Stuecker “Metal Oxide Composites and Structures for Ultra-High Temperature Solar Thermochemical Cycles,” plenary lecture, *Int. Symp. Reactivity of Solids*, Minneapolis, MN, June 3–6, 2007.
35. M.D. Allendorf “Metal Organic Frameworks: Novel Nanoporous Materials for Sensing Applications,” Dept. of Electrical Engineering and Computer Science, University of California, Berkeley, April 18, 2008.
36. J. E. Miller, R. B. Diver, N. P. Siegel, M. D. Allendorf, E. B. Stechel “Sunshine to petrol: Solar thermochemical splitting of carbon dioxide and water,” *ACS 2009 Spring meeting*, Salt Lake City, March 23–26, 2009.
37. M. D. Allendorf “Chemical Detection using Flexible Metal-Organic Frameworks,” *SPIE Defense, Security, and Sensing Conference*, Orlando, FL April 12 – 16, 2009.
38. M. D. Allendorf, R. J. T. Houk, R. J. Bhakta, I. M. B. Nielsen, F. P. Doty “Scintillating Metal Organic Frameworks: A New Class of Radiation Detection Materials,” *MRS 2009 Spring Meeting*, San Francisco, April 13–17, 2009.
39. M. Allendorf, R. Houk, P. Doty, N. Chang, R. Bhakta, B. Jacobs, P. Hesketh “Chemical and radiation sensing using metal-organic frameworks,” Opening Plenary, *MOFCATS Workshop*, Oslo, Norway, June 17–19, 2009.
40. M. D. Allendorf “Applications of Metal-Organic Frameworks Beyond Hydrogen Storage: Way Beyond,” National Institutes of Standards and Technology, August 19, 2009.
41. M. D. Allendorf “Applications of Metal-Organic Frameworks to Chemical and Radiation Detection, Nanoscale Cluster Templating, and Beyond,” *Inorganic Chemistry Lecture Series*, University of California, Berkeley, October 2, 2009.
42. J. Miller, R. Diver, N. Siegel, E. Coker, A. Ambrosini, D. Dedrick, M. Allendorf, G. Kellogg, R. Hogan, E. Stechel, K. Chen “Sunshine to Petrol: A Metal Oxide-Based Thermochemical Route to Solar Fuels,” *Energy Symposiums 2010 of TMS Annual Meeting*, Seattle, February, 2010, Best Paper award.
43. M. Allendorf, V. Stavila, K. C. Kim, D. Sholl “Combining First Principles and Thermodynamic Calculations to Predict Evolution of Impurity Gases from Metal Hydrides,” *2010 ACS Spring meeting*, San Francisco, CA, March 21-25, 2010.
44. M. D. Allendorf “Metal-Organic Frameworks: Versatile Materials for Chemical and Radiation Detection Nanoscale Cluster Templating, and More,” *MESA Technology series*, Sandia National Laboratories, May 6, 2010.
45. M. D. Allendorf “Metal-Organic Frameworks: Versatile Materials for Chemical and Radiation Detection, Nanoscale Cluster Templating, and More,” Dept. of Chemistry, University of California, San Diego, May 14, 2010.
46. M. D. Allendorf, G. H. Evans, B. W. Jacobs, A. H. McDaniel, J. E. Miller, J. Scheffe, A. W. Weimer “Thermodynamic and Kinetic Investigations of Thermochemical Gas Splitting,” ETH, Zurich, Switzerland, July 1, 2010.
47. M. D. Allendorf, G. H. Evans, B. W. Jacobs, A. H. McDaniel, J. E. Miller, J. Scheffe, A. W. Weimer “Kinetics of CO<sub>2</sub> and H<sub>2</sub>O splitting by mixed-metal ferrites: an experimental and computational investigation,” *1st International Conference on Materials for Energy*, Karlsruhe, Germany, July 5–8, 2010.

48. P. L. Feng, F. P. Doty, J. J. Perry, S. T. Meek, M. D. Allendorf "MOF-based Scintillators," *X-Ray, Gamma-Ray, and Particle Technologies; Penetrating Radiation Systems and Applications XI (Conference 7806)*, SPIE Conference, San Diego, August 2–6, 2010.
49. M. D. Allendorf, B. W. Jacobs, R. J. T. Houk, Y. Kobayashi, B. Wiers, J. R. Long, A. A. Talin, P. J. Hesketh, J. H. Lee, A. Venkatasubramanian "Manipulation of MOFs for Device Fabrication," *MOF2010 Conference*, September 5-8, 2010.
50. M. D. Allendorf "Integration of MOF Thin Films with Mechanical Sensors for Chemical Detection," *PITTCON*, Atlanta, GA, March 13–18, 2011.
51. M. D. Allendorf and J. E. Miller "Solar fuel production using thermochemical cycles: a challenging materials problem," Harvard University School of Engineering and Applied Science, April 21, 2011.
52. M. D. Allendorf "Manipulation of MOFs for Device Fabrication," UOP LLC Invitational Lecture Series, Des Plaines, IL, May 4, 2011.
53. M. D. Allendorf "Chemical and Radiation Detection Using Metal-Organic Frameworks," GE Global Research Center June 7-8, 2011, Niskayuna, NY.
54. M. D. Allendorf "Metal-Organic Frameworks (MOFs): Charting a course to device integration," SPIE Nanoeptaxy symposium, San Diego, CA, Aug. 24, 2011.
55. M. D. Allendorf, T. R. Zeitler, J. A. Greathouse "Metal-organic frameworks for greenhouse gas detection," *ACS Fall 2011 Meeting*, Denver, CO, Aug. 29, 2011.
56. M. D. Allendorf, A. H. McDaniel, J. E. Miller, E. N. Coker, A. Ambrosini, T. Aston, A. Weimer, J. Scheffe "Solar Fuel Production Using Thermochemical Cycles: A Challenging Materials Problem," *Fall Meeting of The Electrochemical Society*, Boston, MA, October 9-14, 2011.
57. M. D. Allendorf "Nano-to-Macro Materials Solutions to Renewable Energy Production and Storage," Dept. of Mech. Eng., Univ. Maryland, College Park, Oct. 14, 2011.
58. M. D. Allendorf "Luminescent metal-organic frameworks (MOFs): a nanolaboratory for photophysics," MIT Center for Excitonics Lecture Series," Cambridge, Massachusetts, February 7, 2012.
59. M. D. Allendorf, A. H. McDaniel, A. Ambrosini, E. N. Coker, J. E. Miller, E. B. Stechel "Solar-Driven Fuel Production Using Metal Oxide Thermochemical Cycles," *Materials Challenges in Alternative & Renewable Energy 2012 (MCARE)*, Clearwater, FL, February 26 – March 1, 2012.
60. M. D. Allendorf "Tuning Thermodynamics and Kinetics of Complex Metal Hydrides Using Ordered Nanoporous Templates," *Spring 2012 MRS (hydrogen storage)*, San Francisco, CA, April 9-13, 2012.
61. M. D. Allendorf "Connecting Structure with Function: MOFs for Chemical and Radiation Detection," *DFG Priority Program on MOFs, Topical Workshop for PhD Students: MOF-Based Chemical Sensors*, Munich, Germany, March 12–13, 2012.
62. M. D. Allendorf "The Power of Empty Space," *Valley Study Group*, Pleasanton, CA, June 13, 2012.
63. M. D. Allendorf "Research Connections with Sandia National Laboratories," *University-Government-Industry Micro-Nano Conference*, July 9-11, 2012, Berkeley, CA.
64. M. D. Allendorf, M. Foster, D. Gough, T. N. Lambert, K. Leong, S. T. Meek, E. D. Spoeke, B. Wong "Controlling donor-acceptor interfaces in excitonic devices using nanoporous metal-organic framework templates," *ACS Fall 2012 Meeting*, Philadelphia, PA, August 20–23, 2012.
65. M. D. Allendorf "The Power of Empty Space: Manipulating MOFs for Device Applications," Dept. of Chemistry, Washington University, St. Louis, MO Oct. 25, 2012.
66. M. D. Allendorf "The Power of Empty Space: Manipulating MOFs for Device Applications," Dept. of Physics, University of Missouri, St. Louis, MO, Oct. 26, 2012.
67. M. D. Allendorf "Creating donor-acceptor interfaces for excitonic devices using nanoporous metal-organic frameworks," *Electronic Materials and Applications 2013 Conference*, Orlando, FL, January 23-25, 2013.
68. M. D. Allendorf "Manipulating MOFs for Nanoparticle, Thin Film, and Device Fabrication," University of South Florida, Tampa, FL, January 25, 2013.
69. V. Stavila, M. D. Allendorf "Metal-Organic Frameworks as Nanoreactors for Reversible De/Rehydrogenation Reactions," *245<sup>th</sup> ACS National Meeting*, New Orleans, LA, April 7-11, 2013.

70. M. D. Allendorf, J. M. Denning, J. A. Greathouse, A. L. Robinson, V. Stavila, T. R. Zeitler, I. Ellern, P. J. Hesketh "Integrating MOFs with MEMS devices for chemical sensing," *245<sup>th</sup> ACS National Meeting*, New Orleans, LA, April 7-11, 2013.
71. M. D. Allendorf, "Nanoporosity and the Welcome Guest: Developing Metal-Organic Frameworks for Electronic Device Applications," Dept. of Materials Science, Univ. of Cambridge, Cambridge, U.K. Sept. 9, 2013.
72. M. D. Allendorf, A. A. Talin, J. A. Greathouse, T. N. Lambert, E. D. Spörke, V. Stavila, B. M. Wong "The Power of Empty Space: Metal-Organic Frameworks as Electronic Materials," *EuroMat 2013*, Seville, Spain, Sept. 9 – 13, 2013.

### **Patents**

1. S. F. Rice and M. D. Allendorf "Apparatus for measuring the concentration of a species at a distance," U. S. Patent 7027150, issued April 11, 2006.
2. "Hybrid Metal Organic Scintillator Materials System and Particle Detector," US Patent 7,985,868.
3. M. D. Allendorf and P. J. Hesketh "Method and Apparatus for Detecting an Analyte," US 8,065,904B1.