

David S. Mebane, Ph.D.

Assistant Professor

Department of Mechanical and Aerospace Engineering

West Virginia University

ORISE Faculty Fellow

National Energy Technology Laboratory

Morgantown, WV, USA

Education

Ph.D., Materials Science and Engineering, Georgia Institute of Technology, 2007

M.S., Materials Science and Engineering, Georgia Institute of Technology, 2004

B.A., Mechanical Engineering/History, Rice University, 1996

Peer-Reviewed Articles

Total citations: 672 (Google Scholar) / 435 (ISI)

h-factor: 15 (Google Scholar) / 12 (ISI)

1. A. F. Zurhelle, X. Tong, A. Klein, D. S. Mebane and R. A. De Souza, "A space-charge treatment of the increased concentration of reactive species at the surface of a ceria solid solution," *Angewandte Chemie*, **56** (2017) 14516.
2. G. F. Brunello, W. K. Epting, K. de Silva, P. A. Salvador, S. Litster, H. O. Finklea, Y.-L. Lee, K. Gerdes and D. S. Mebane, "Quantitative interpretation of impedance spectroscopy data on porous LSM electrodes using x-ray computed tomography and Bayesian model-based analysis," *Physical Chemistry Chemical Physics*, **19** (2017) 25334.
3. J. Zhu, J. Wang, D. S. Mebane and S. S. Nonnenmann, "*In-situ* surface potential evolution along Au/Gd: CeO₂ electrode interfaces," *APL Materials*, **5** (2017) 042503.
4. K. Li, P. Mahapatra, K. S. Bhat, D. C. Miller and D. S. Mebane, "Multi-scale modeling of an amine sorbent fluidized bed adsorber with dynamic discrepancy reduced modeling," *Reaction Chemistry and Engineering*, **2** (2017) 550.
5. K. S. Bhat, D. S. Mebane, C. B. Storlie and P. Mahapatra, "Upscaling uncertainty with dynamic discrepancy for a multi-scale carbon capture system," *Journal of the American Statistical Association*, (2017) in press.
6. X. Tong and D. S. Mebane, "Kinetic modeling of near-interface defect segregation during thermal annealing of oxygen-conducting solid electrolytes," *Solid State Ionics*, **299** (2017) 78.
7. K. Li, J. D. Kress and D. S. Mebane, "The mechanism of CO₂ adsorption under dry and humid conditions in mesoporous silica-supported amine sorbents," *The Journal of Physical Chemistry C*, **120** (2016) 23683.

8. D. S. Mebane and R. A. De Souza, "A generalised space-charge theory for extended defects in oxygen-ion conducting electrolytes: from dilute to concentrated solid solutions," *Energy & Environmental Science*, **8** (2015) 2935.
9. D. S. Mebane, "A variational approach to surface cation segregation in mixed conducting perovskites," *Computational Materials Science*, **103** (2015) 231.
10. H. Abernathy, H. O. Finklea, D. S. Mebane, X. Song, Y. Chen and K. Gerdes, "Examination of the mechanism for the reversible aging behavior at open circuit when changing the operating temperature of $(\text{La}_{0.8}\text{Sr}_{0.2})_{0.95}\text{MnO}_3$ electrodes," *Solid State Ionics*, **272** (2015) 144.
11. J. Blair and D. S. Mebane, "A Bayesian approach to electrical conductivity relaxation and isotope exchange / secondary ion mass spectrometry," *Solid State Ionics*, **270** (2015) 47.
12. D. C. Miller, M. Syamlal, D. Mebane, C. Storlie, D. Bhattacharyya, N. V. Sahinidis, D. Agarwal, C. Tong, S. E. Zitney, A. Sarkar, X. Sun, S. Sundaresan, E. Ryan, D. Engel and C. Dale, "Carbon Capture Simulation Initiative: A case study in multiscale modeling and new challenges," *Annual Review of Chemical and Biomolecular Engineering*, **5** (2014) 301.
13. M. Gong, R. S. Gemmen, D. S. Mebane, K. Gerdes and X. Liu, "Simulation of surface potential-driven ORR kinetics on SOFC cathode with parallel reaction pathways," *Journal of the Electrochemical Society*, **161** (2014) F344.
14. D. S. Mebane, J. D. Kress, C. B. Storlie, D. J. Fauth, M. L. Gray and K. Li, "Transport, zwitterions and the role of water for CO_2 adsorption in mesoporous silica-supported amine sorbents," *Journal of Physical Chemistry C*, **117** (2013) 26617.
15. D. S. Mebane, K. S. Bhat, J. D. Kress, D. J. Fauth, M. L. Gray, A. Lee and D. C. Miller, "Bayesian calibration of thermodynamic models for the uptake of CO_2 in supported amine sorbents using *ab initio* priors," *Physical Chemistry Chemical Physics*, **15** (2013) 4355.
16. H. W. Abernathy, H. O. Finklea, D. S. Mebane, X. Chen, K. Gerdes and M. D. Salazar-Villalpando, "Reversible aging behavior of LSM electrodes at open circuit," *Journal of Power Sources*, **216** (2012) 11.
17. D. S. Mebane and J. Maier, "D.C. ionic conductivity in silver chloride, revisited," *Physical Chemistry Chemical Physics*, **12** (2010) 2478.
18. D. S. Mebane and J.-H. Wang, "A general method of solution for the cluster variation method in ionic solids, with application to diffusionless transitions in yttria-stabilized zirconia," *Journal of Statistical Physics*, **139** (2010) 727.
19. M. Lynch, D. S. Mebane, Y. Liu, M. L. Liu, "Triple phase boundary and surface transport in a numerical mixed conducting thin film patterned electrode model," *Journal of the Electrochemical Society*, **155** (2008) B635.
20. D. S. Mebane, Y. Liu and M. L. Liu, "Refinement of the bulk defect model for $\text{La}_x\text{Sr}_{1-x}\text{MnO}_{3\pm\delta}$," *Solid State Ionics*, **178** (2008) 1950.
21. Y. M. Choi, D. S. Mebane, M. C. Lin and M. L. Liu, "Oxygen reduction for LaMnO_3 -based cathode materials in solid oxide fuel cells," *Chemistry of Materials*, **19** (2007) 1690.

22. Y. M. Choi, J. H. Wang, D. S. Mebane and M. L. Liu, "Continuum and quantum-chemical modeling of oxygen reduction on the cathode in a solid oxide fuel cell," *Topics in Catalysis*, **46** (2007) 386.
23. D. S. Mebane, Y. Liu and M. L. Liu, "A two-dimensional model and numerical treatment for mixed conducting thin films," *Journal of the Electrochemical Society*, **154** (2007) A421.
24. R. Das, D. S. Mebane, E. Koep and M. L. Liu, "Modeling of patterned mixed-conducting electrodes and the importance of sheet resistance at small feature sizes," *Solid State Ionics*, **178** (2007) 249.
25. D. S. Mebane and M. L. Liu, "Classical, phenomenological analysis of the kinetics of reactions at the gas-exposed surface of mixed ionic electronic conductors," *Journal of Solid State Electrochemistry*, **10** (2006) 575.
26. E. Koep, D. S. Mebane, R. Das, C. Compson and M. L. Liu, "The characteristic thickness for a $\text{La}_{0.8}\text{Sr}_{0.2}\text{MnO}_3$ electrode," *Electrochemical and Solid State Letters*, **8** (2005) A592.
27. D. S. Mebane and R. A. Gerhardt, "Interpreting impedance response of silicon carbide whisker / alumina composites through microstructural simulation," *Journal of the American Ceramic Society*, **89** (2006) 538.
28. D. S. Mebane, A. M. Gokhale and R. A. Gerhardt, "Trivariate, stereological length-radius-orientation unfolding derived and applied to alumina-silicon carbide whisker composites," *Journal of the American Ceramic Society*, **89** (2006) 620.
29. D. S. Mebane, S. I. Lieberman, A. M. Gokhale and R. A. Gerhardt, "Bivariate stereological unfolding procedure for randomly oriented chopped fibers or whiskers," *Acta Materialia*, **53** (2005) 4943.

Patents

1. M. L. Liu, M. F. Liu, L. F. Nie, D. S. Mebane, L. C. Wilson and W. Surdoval, "Solid oxide fuel cells having porous cathodes infiltrated with oxygen-reducing catalysts," U.S. Patent no. 8802316, 2014.

Technical Presentations and Conference Proceedings

Invited

1. D. S. Mebane, "Data-Driven Models in Solid State Electrochemistry," Florida International University Graduate Seminar, November 2018.
2. D. S. Mebane, "Poisson-Cahn: A Space Charge Theory for Dilute and Concentrated Systems," AiMES 2018, Cancún, Mexico, October 2018.
3. D. S. Mebane, A. H. Romero and P. Tavazohi, "Intrusive Uncertainty Quantification (and a More Accurate Functional) in Density Functional Theory," National Institute of Standards and Technology, April 2018.

4. D. S. Mebane, "Dynamic Discrepancy: Intrusive Methods for Getting More Science into Industrial Models," SIAM Conference on Uncertainty Quantification, Garden Grove, CA, April 2018.
5. D. S. Mebane, "The electrochemical interface: Progress toward a unified continuum theory for dilute and concentrated systems," NETL Fuel Cell Group Seminar, December 2017.
6. D. S. Mebane, "The electrochemical interface: Progress toward a unified continuum theory for dilute and concentrated systems," MRS Fall Meeting, Boston, November 2017.
7. D. S. Mebane, A. H. Romero and K. X. Kocan, "The case for intrusive uncertainty quantification in density functional theory," TMS, San Diego, March 2017.
8. D. S. Mebane, "The Poisson-Cahn space charge theory for concentrated solid electrolytes," EMA, Orlando, January 2017.
9. D. S. Mebane, "Bayesian calibration and predictive modeling through data," CENAM, Queretaro, Mexico, July 2016.
10. D. S. Mebane, "Poisson-Cahn: A space charge theory for concentrated solid electrolytes," E-MRS Spring Meeting, Lille, France, May 2016.
11. D. S. Mebane, "Poisson-Cahn: A space charge theory for concentrated solid electrolytes," RWTH Aachen University, October 2015.
12. D. S. Mebane, "Surface-mediated spinodal in perovskite oxides," Gordon Research Conference on Ceramics, Mt. Holyoke College, July 2014.
13. D. S. Mebane, K. S. Bhat, J. D. Kress, D. J. Fauth and M. L. Gray, "Uncertainty quantification in chemistry sub-models," NETL 2012 Workshop on Multiphase Flow Science, Morgantown, May 2012.
14. D. S. Mebane, K. S. Bhat, J. D. Kress, D. J. Fauth and M. L. Gray, "Kinetic model for silica supported amines with uncertainty quantification," Carbon Capture, Utilization and Sequestration, Pittsburgh, May 2012.
15. K. S. Bhat, D. S. Mebane, J. D. Kress and J. R. Wendelberger, "Uncertainty quantification in solid sorbent models," Carbon Capture Simulation Initiative Industry Advisory Board Workshop, Washington, D.C., April 2012.
16. "Solid sorbent modeling," Carbon Capture Simulation Initiative Industry Advisory Board Workshop, Morgantown, September 2011.
17. "Solid sorbent modeling for the Carbon Capture Simulation Initiative," NETL 2011 Workshop on Multiphase Flow Science, Pittsburgh, August 2011.
18. "Theory and numerical methods in solid state ionics," National Energy Technology Laboratory, Morgantown, August 2010.
19. "Equilibrium and transport beyond the ideal in LSM," RWTH Aachen University, May 2009.

20. D. S. Mebane and J. Maier, "From dilute electrolytes to superionic solids: a discussion of the Coulomb interaction," *Arbeitsbesprechung*, Max Planck Institute for Solid State Research, July 2008.
21. D. S. Mebane and J. Maier, "From dilute electrolytes to superionic solids: a discussion of the Coulomb interaction," International symposium on defects, Transport and Related Phenomena, Materials Science and Technology, Pittsburgh, September 2008.

Contributed

1. X. Tong, D. S. Mebane, D. R. Diercks and B. Gorman, "Bayesian Calibration of a Poisson-Cahn Model in Predicting Quantification of Composition at Grain Boundaries in Highly-Doped Ceria," MRS Fall Meeting, Boston, 2017.
2. A. Ostace, D. Bhattacharyya, K. X. Kocan and D. S. Mebane, "Data-driven model building of zeolite adsorption processes with uncertainty quantification and propagation to dynamic simulations of CO₂ adsorption in a fixed bed reactor," AIChE Annual Meeting, Minneapolis, 2017.
3. G. F. Brunello and D. S. Mebane, "Bayesian model based analysis of impedance spectroscopy on LSM cathodes," SSI, Padua, Italy, 2017.
4. D. S. Mebane, X. Tong, R. A. De Souza, D. Diercks and B. Gorman, "A theory of co-accumulation and depletion at grain boundaries in acceptor-doped ceria," SSI, Padua, Italy, 2017.
5. A. Ostace, D. Bhattacharyya, K. Kocan and D. S. Mebane, "Dynamic modeling with uncertainty quantification of CO₂ adsorption in a fixed bed reactor," AIChE Annual Meeting, San Francisco, 2016.
6. D. S. Mebane, "Dynamic discrepancy reduced modeling: Overview and applications," AIChE Annual Meeting, San Francisco, 2016.
7. X. Tong and D. S. Mebane, "Kinetic modeling of near-interface defect segregation during thermal annealing of oxygen-conducting solid electrolytes," E-MRS Spring Meeting, Lille, France, 2016.
8. J. D. Kress, K. Li, D. S. Mebane, P. Mahapatra and K. S. Bhat, "Integration of high-fidelity CO₂ sorbent models at the process scale using dynamic discrepancy," CO₂ Summit, Santa Ana Pueblo, NM, 2016.
9. E. Ford, F. V. Lima and D. S. Mebane, "Multi-scale chemical process modeling with Bayesian nonparametric regression," AIChE Annual Meeting, Salt Lake City, 2015.
10. K. Li, D. S. Mebane and P. Mahapatra, "Integration of high-fidelity CO₂ sorbent models at the process scale using dynamic discrepancy," AIChE Annual Meeting, Salt Lake City, 2015.
11. J. C. Eslick, C. Tong, B. Ng, A. Lee, A. W. Dowling, D. S. Mebane, Y. Chen and D. C. Miller, "Optimization under uncertainty with rigorous process models," AIChE Annual Meeting, Salt Lake City, 2015.

12. D. S. Mebane and X. Tong, "Modeling a surface-mediated spinodal in doped mixed conducting perovskites," 20th International Conference on Solid State Ionics, Keystone, CO, 2015.
13. G. F. Brunello, W. K. Epting, S. Litster, P. A. Salvador, H. O. Finklea, K. R. Gerdes, J. De Silva and D. S. Mebane, "Nano-CT enabled, Bayesian model-based analysis of impedance data for a porous, lanthanum strontium manganate cell," 20th International Conference on Solid State Ionics, Keystone, CO, 2015.
14. D. S. Mebane, K. S. Bhat, C. B. Storlie and P. Mahapatra, "Multi-scale modeling with dynamic discrepancy," AIChE Annual Meeting, Atlanta, 2014.
15. K. Li, J. D. Kress and D. S. Mebane, "New diffusive intermediates for CO₂ adsorption in silica-supported amine sorbents," AIChE Annual Meeting, Atlanta, 2014.
16. E. Ford, F. Lima and D. S. Mebane, "A Bayesian approach to reduced order modeling in catalytic steam reformation," American Institute of Chemical Engineers Annual Meeting, Atlanta, 2014.
17. D. S. Mebane, A. Koneru and T. Musho, "Thermoelectricity in cobalt-containing spinel nanocomposites," Gordon Research Conference on Ceramics, Mt. Holyoke College, July 2014.
18. D. S. Mebane, A. Koneru and T. Musho, "First principles calculation of thermoelectric properties in doped spinels with uncertainty quantification," Materials Research Society Spring Meeting, San Francisco, 2014.
19. D. S. Mebane and J. Blair, "Bayesian analysis of electrical conductivity relaxation experiments," Materials Research Society Spring Meeting, San Francisco, 2014.
20. D. S. Mebane, K. S. Bhat and C. B. Storlie, "Uncertainty quantification in multi-scale models of chemical processes," CECAM/Psi-k Conference on Multi-Scale Modeling, Cap Roig, Spain, 2013.
21. D. S. Mebane, K. S. Bhat and C. B. Storlie, "Multi-scale modeling with generalized dynamic discrepancy," SIAM Annual Meeting, San Diego, 2013.
22. D. S. Mebane, "Bayesian methods in multiscale modeling," Materials Research Society Fall Meeting, Boston, 2012.
23. D. S. Mebane, C. B. Storlie, J. D. Kress, L. M. Moore, D. J. Fauth and M. L. Gray, "The importance of transport processes in silica-supported, polyethyleneimine-impregnated CO₂ sorbents," AIChE Annual Meeting, Pittsburgh, 2012.
24. D. S. Mebane, K. S. Bhat, J. D. Kress, D. J. Fauth, M. L. Gray, A. Lee and D. C. Miller, "Bayesian methods in multiscale modeling," AIChE Annual Meeting, Pittsburgh, 2012.
25. D. S. Mebane, K. S. Bhat, L. M. Moore, J. D. Kress, D. J. Fauth and M. L. Gray, "Solid sorbent modeling in the Carbon Capture Simulation Initiative," MRS Spring Meeting, San Francisco, 2012.

26. D. S. Mebane, D. J. Fauth and M. L. Gray, "A rigorous yet scalable kinetic model for the uptake of CO₂ by silica-supported, PEI-impregnated sorbents," International Pittsburgh Coal Conference, Pittsburgh, 2011.
27. A. Lee, D. S. Mebane and D. J. Fauth, "A model for the adsorption kinetics of CO₂ on amine-impregnated, mesoporous sorbents in the presence of water," International Pittsburgh Coal Conference, Pittsburgh, 2011.
28. "The cluster variation method in solid state ionics," European Materials Research Society, Strasbourg, 2010.
29. D. S. Mebane and J. Maier, "Mean-field approaches for Coulomb interactions and bound pairs in silver chloride," Solid State Ionics, Toronto, 2009.
30. M. E. Lynch, D. S. Mebane and M. L. Liu, "Numerical continuum modeling and simulation of mixed-conducting thin film and patterned electrodes," American Ceramic Society, Cocoa Beach, 2009.
31. D. S. Mebane, Y. Liu and M. L. Liu, "A low-temperature bulk model for La_xSr_{1-x}MnO_{3±δ}," European Ceramic Society, Berlin, 2007.
32. D. S. Mebane and M. L. Liu, "Modeling of MIEC cathodes: the effect of sheet resistance," American Ceramic Society, Cocoa Beach, 2006.
33. D. S. Mebane, A. M. Gokhale and M. L. Liu, "Explicit computational investigations on the effect of microstructure in solid oxide fuel cell electrodes," Microscopy and Microanalysis, Honolulu, 2005.
34. D. S. Mebane and R. A. Gerhardt, "Impedance response of alumina silicon carbide whisker composites," TMS, San Francisco, 2005.
35. D. S. Mebane, A. M. Gokhale and R. A. Gerhardt, "The effect of microstructural interconnectivity on the resistivity of Al₂O₃-SiC_w composites," NUMIFORM, Columbus, 2004.

Graduated Students

1. Xiaorui Tong, Ph.D., Materials Science and Engineering, 2018
2. Ahmed Nirjhar Alam, M.S., Mechanical Engineering, 2018
3. Alejandro Mejia, M.S., Aerospace Engineering, 2017 (current grad student)
4. Kuijun Li, Ph.D., Mechanical Engineering, 2016 (Hessaire)
5. Brian Logsdon, M.S., Mechanical Engineering, 2016 (West Virginia Robotic Technology Center)
6. Evan Ford, M.S. Mechanical Engineering, 2015 (Volvo USA)
7. Joshua Blair, M.S. Mechanical Engineering, 2014 (Kanawha County Schools)

Funding

- “Collaborative Research: Combining Models and Experiment for Quantitative Characterization of Electrocatalytic Carbon Dioxide Reduction on Doped Ceria,” National Science Foundation (Catalysis Program), \$190k, PI (sole investigator), 2017
- “Dynamic Discrepancy Reduced Modeling for Adaptive, Multi-Model Nonlinear Model Predictive Control,” ACS Petroleum Research Fund (Young Investigator Award), \$110k, PI (2 investigators), 2016
- “Commercialization and Enhancement of CCSI PSE Models and Tools,” Process Systems Enterprise, \$230k, co-PI (2 investigators), 2015
- “Carbon Capture Simulation Initiative WVU Subcontract,” University of California (Lawrence Berkeley National Laboratory), \$558k, PI (3 investigators), 2014
- “Carbon Capture Simulation Initiative Task 2 Support – 2nd Generation Solid Sorbent Sub-model and Fitting Tool,” U.S. Department of Energy (NETL), \$91k, PI (sole investigator), 2013
- “Bayesian Statistical Model of Degradation,” U.S. Department of Energy (NETL), \$76k, PI (sole investigator), 2013
- “CCSI Element 1: Basic Data and Models,” U.S. Department of Energy (NETL), \$159k, PI (sole investigator), 2012

Service

- Symposium Co-Organizer, 2018 E-MRS Annual Meeting
- Session Chair, 2016 AIChE Annual Meeting
- Session Co-Chair, 2015 AIChE Annual Meeting
- MRS Congressional Visits Day Team Member, 2015.
- Reviewer, *Solid State Ionics*, *Journal of the Electrochemical Society*, *Journal of Physical Chemistry*, *Energy and Fuels*, *Physical Chemistry Chemical Physics*, *Computational Materials Science*, *Nanoscale*, *Nano Letters*, *AIChE Journal*, *Acta Materialia*, *Electrochimica Acta*, *Environmental Science and Technology*, *Journal of the American Ceramic Society*, *Journal of Materials Chemistry A*, *Langmuir*, *Nature Partner Journals Computational Materials Science*, *Nature Materials*
- Member, Materials Research Society, Society for Industrial and Applied Mathematics, International Society for Solid State Ionics, The Electrochemical Society

Awards

- R&D 100 Award (CCSI Toolset), 2016
- NSF International Research Fellowship Program, 2008-2010
- NSF International Travel Award, 2007, 2013
- Georgia Institute of Technology Boeing Fellow, 2005-2007
- Best Master's Thesis, School of Materials Science and Engineering, Georgia Tech, 2004

Work History

- 2018-present** Associate Professor, Department of Mechanical and Aerospace Engineering, West Virginia University, Morgantown, WV
- 2012-2018** Assistant Professor, Department of Mechanical and Aerospace Engineering, West Virginia University, Morgantown, WV
- 2015-present** ORISE Faculty Fellow, National Energy Technology Laboratory, Morgantown, WV
- 2010-2012** ORISE Postdoctoral Fellow, Computational Science Division, National Energy Technology Laboratory, Morgantown, WV
- 2008-2010** NSF Postdoctoral Fellow, Max Planck Institute for Solid State Research, Stuttgart, Germany
- 2002-2007** Graduate Student, Georgia Institute of Technology, Atlanta, GA
- 5-8/2003** Analyst, Georgia Tech Research Corporation Technology Transfer Office
- 2001-2002** Executive Recruiter, Leader Institute, Marietta, GA
- 2000-2001** Executive Recruiter, Self-employed, New Orleans, LA
- 1998-2000** Executive Recruiter, MSI International, New Orleans, LA