

## Marius STAN, Ph.D.

**Retired. Former Senior Scientist, Program Leader, Center Director, National Technical Director.**

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**Personal statement:** I retired in June 2021 to have more control over my time and pursue projects in Artificial Intelligence, literature, and cinematography. A physicist and chemist by training and a computational scientist by profession, I consider myself a creator, leader, and contributor to society. As Senior Scientist and Program Leader for Intelligent Materials Design, I promoted an innovative approach that uses elements of artificial intelligence, such as machine learning, natural language processing and computer vision, to understand and optimize multi-component materials for energy, manufacturing, and national security applications. In 2000, I created and led the research team that pioneered the concept of “multi-scale modeling and simulation.” Our methodology – which has been adopted by the international community – couples theoretical and computational methods that operate at different length and time scales, from atomistic, to meso-scale, to continuum. I feel privileged to be the co-author of some of the first papers on uncertainty quantification of phase diagrams and on phase field simulations of irradiation effects in materials. From 2013 to 2015, I managed DOE national modeling and simulation programs of over \$50 mil/year total budget and developed institutional, national, and international vision and strategic plans for scientific computing. As manager of organizations of 80 to 100 people with budgets of 15-25 mil/year, I set vision and medium/long term goals and increased the funding at a rate of 5-10%/year. Several projects I created, such as the OECD/NEA multi-scale modeling and simulation working party or the materials modeling of nuclear fuels international workshop, are now prestigious international activities. Throughout my career, I promoted a safe, secure, and diverse environment. I also promoted the synergy between science, art, and society via a series of presentations at universities, cultural centers, public libraries, and schools in Chicago and other cities across the world. Happiness is living above expectations.

### EDUCATION

**1997, Ph.D. (Chemistry)**, Romanian Academy, Institute of Physical Chemistry, Bucharest, Romania.

**1986, B.S. (Physics)**, University of Bucharest, Bucharest, Romania.

### PROFESSIONAL EXPERIENCE

2018-2021, **Senior Scientist and Program Leader**, Intelligent Materials Design, Applied Materials Division, Argonne National Laboratory (ANL).

- Improved the understanding, prediction and design of multi-component materials by using elements of artificial intelligence, machine learning, computer vision, and multi-scale computer simulations.
- Led the development of high performance, multi-physics computational tools for applications in materials design, advanced manufacturing, and advanced computing.
- Participated in defining goals and vision for intelligent material and process design at local (ANL), national (DOE, DOC, DOD) and international (OECD) levels.

2013-2021, **Senior Fellow**, Northwestern-Argonne Institute for Science and Engineering (NAISE), Northwestern Univ.

- Improved uncertainty evaluation of phase stability diagrams of multicomponent systems by developing thermodynamic models and using Bayesian analysis and machine learning.
- Designed improved materials at the Center for Hierarchical Materials Design (ChiMaD).
- Prepared a course on computational materials science, with an emphasis on multi-scale methods, experimental validation, and material design.

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2011-2021, **Senior Fellow**, Consortium for Advanced Science and Engineering (CASE), Univ. of Chicago.

- Improved the analysis of large data sets using artificial intelligence and machine learning.
- Prepared a course on computational science, with an emphasis on multi-scale and coupled physics.

2017-2018, **Interim Director**, Systems Science Center, Global Security Sciences Division, ANL.

- Led and managed the Systems Science Center. The center developed integrated computational and analytical solutions that increased the understanding of physical, social, economic, and technological interrelationships; anticipated future conditions; and supported decision making and policy making in complex environments.

2015-2017, **Group Leader**, Complex Physical Systems Group, Global Security Science Division, ANL.

- Created and led the “Complex Physical Systems” Group in the Systems Science Center. The group advances the understanding and prediction of complex systems that are governed by the laws of physical sciences for energy, defense, and national security applications.
- Led the development of multi-scale and multi-physics computational models using elements of artificial intelligence such as machine learning, natural language processing and immersive visualization.

2013-2015, **Senior Advisor and National Technical Director**, Department of Energy (DOE), Office of Nuclear Energy, NE-1.

- Developed institutional, national, and international vision and strategic plans for advanced modeling and simulation in support of nuclear energy applications.
- Interfaced with similar programs in DOE: Office of Science and National Nuclear Security Agency.
- Managed the Nuclear Energy Advanced Modeling and Simulation (NEAMS) program.
- Increased budget by 50% over two years to a level over \$25 mil/year.
- Introduced the concept of High Impact Problems (HIPs) and increased the visibility of the program.
- Improved the work environment and attracted high quality model and software developers.
- Coordinated research activities with other DOE-NE programs, especially the Consortium for Advanced Simulation of Light Water Reactors (CASL).

2010-2016, **Senior Scientist**, Nuclear Energy Division, ANL.

- Developed theory and models of physical systems and materials that are “heterogeneous by design.”
- Improved the understanding of coupled heat transport, species diffusion, and thermal expansion of ceramics and alloys by performing Finite Element Method (FEM) simulations.
- Designed materials for energy storage (Li-O) and electronics (Hf-Si-O) by developing free energy models and running Phase Field (PF) simulations of microstructure evolution.
- Improved the understanding and prediction of defect formation and evolution in oxides for energy applications (U-O, Pu-O) and oxides for electronics (Ce-O, Hf-O) by developing force fields and performing Density Functional Theory (DFT) and Molecular Dynamics (MD) simulations.

2007-2010, **Deputy Group Leader**, Computational Physics Group, Los Alamos National Laboratory (LANL).

- Provided scientific leadership and programmatic/administrative management to group of 70-90 including software developers for the *RoadRunner* supercomputer and computational climate simulation experts.
- Set vision and goals for the group and increased funding at a rate of 5%/year.
- Developed international strategy for the Organization for Economic Cooperation and Development (OECD), the Nuclear Energy Agency (NEA) that resulted in a working party on multi-scale models

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and simulation for nuclear energy and five international expert groups involving sixteen OECD countries.

2006-2007, **Deputy Group Leader**, Structure-Properties Relations Group, Materials Science and Technology Division, LANL.

- Participated in management of group of over one hundred, integrating experiments, theory, and computation.
- Set vision and goals for the group and increased funding at a rate of 10%/year.
- Performed FEM simulations of coupled heat conduction, species diffusion, and thermal expansion in alloys and ceramics.

2005-2006, **Team Leader**, Thermodynamics of Materials Team, Structure-Properties Relations Group, Materials Science and Technology Division, LANL.

- Created and led a computational and experimental thermodynamics of materials team of sixteen staff members, postdocs, and students.
- Performed advanced FEM simulations (COMSOL) of transport in nuclear fuel elements.

1999-2005, **Technical Staff Member**, Materials Science and Technology Division, LANL.

- Pioneered the concept of “multi-scale models and simulations” and the associated methodology of coupling theoretical and computational methods that operate at specific lengths and time scales, from atomistic, to meso-scale, to continuum.
- Successfully applied the methodology to actinide-based materials such as plutonium-gallium alloys (Pu-Ga) and uranium oxide (UO<sub>2</sub>). This methodology is now being widely used in studies of actinides and other materials.
- Developed MD and CALPHAD models of phase stability of alloys such as Al-Cu and Pu-Ga that increased the understanding and control of ageing in materials.
- Developed free energy models and PF simulations of microstructure evolution in alloys (Pu-Ga) and ceramics (UO<sub>2</sub>, PuO<sub>2</sub>) that created a novel approach to understanding and controlling meso-scale effects.
- Designed and coded components of the thermal transport and phase-change module of the finite volume, multi-physics software TRUCHAS, including nucleation and growth of new phases, that significantly improved the simulations of casting.
- Validated models and simulations using X-ray diffraction (XRD), Differential Thermal Analysis (DTA), Differential Scanning Calorimetry (DSC) and Scanning Electron Microscopy (SEM).
- In 2002 created the Materials Models and Simulations for Nuclear Fuels (MMSNF) workshop series that made “multi-scale models and simulations of nuclear fuels” a widely use scientific methodology.

1997-1999, **Postdoctoral Research Associate**, Materials Science and Technology Division, LANL.

- Developed mathematical models and calculated phase stability (CALPHAD) of multi-component, actinide-based oxides such as Pu-Ga-O.
- Performed experimental validation using DSC, XRD, SEM and TEM.

1989-1997, **Research Scientist**, Institute of Physical Chemistry, Bucharest, Romania.

- Developed mathematical models of thermo-chemical properties and calculated phase stability (CALPHAD) of multi-component ceramics such as Al-Mg-Ti-O and Sn-Sb-Cu-O.
- Validated the models using DSC, DTA, XRD, and SEM experimental data.

1986-1989, **Research Scientist**, ROFEP S. A., Urziceni, Romania.

- Developed mathematical models of thermodynamic properties of ceramics such as Ba(Zn)-Fe-O and Mg-Fe-O.

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- Performed experimental validation using DSC, DTA, XRD, and SEM.

### TEACHING EXPERIENCE

2001-2003, **Adjunct Professor**, University of New Mexico, Albuquerque, NM.

- Taught Physical Chemistry (Quantum Mechanics, Statistical Mechanics, and Thermodynamics) at undergraduate and graduate levels; emphasized the role of experiment, theory, and computation.

### PROFESSIONAL SERVICE

- Founder and Honorary Chair of the “Multiscale Modeling and Simulation of Nuclear Fuels (MMSNF)” workshop series. Started in 2002, the workshop brings together scientists and engineers from all over the world to discuss and advance scientific, engineering, and computational methods.
- Founder and Past Chair of the OECD-Nuclear Energy Agency (NEA) Working Party on “Multi-Scale Modelling of Fuels and Structural Materials for Nuclear Systems.” More than eighteen countries are represented in this working group that creates and publishes State of the Art reports.
- Past Chair of the Scientific Advisory Committee of the “F-BRIDGE” European Community project on advanced nuclear fuels for the new generation nuclear reactors.
- Past Chair of the Scientific Advisory Committee of the U. S. Department of Energy Frontier Research Center (EFRC) on “Materials Science of Nuclear Fuels.”
- Past Member of the Board of Directors of MaRIE (Matter Radiation Interaction in Extremes) signature facility.
- Member of the Alloy Phase (Diagram) Committees of the Metals and Materials Society (TMS) and the Materials Information Society (ASM).
- Member of the American Physical Society (APS) and the American Nuclear Society (ANS).
- Key-Reader and Member of the Editorial Boards of the Materials Theory, Metallurgical and Materials Transactions-A, Journal of Nuclear Materials, and Journal of Phase Diagrams journals.

### AWARDS AND HONORS

- Doctor Honoris Causa, Politehnica University of Bucharest, Romania, 2018
- Outstanding Postdoctoral Mentor, Argonne National Laboratory, 2017
- Honorary Citizen of the city of Urziceni, Romania, 2017
- Appreciation Award from the U. S. A. Department of Energy, for “Significant contributions to the Office of Nuclear Energy’s Advanced Modeling and Simulations Program,” 2015
- U. S. A. Department of Energy “Pollution Prevention Award” for innovative science and technology in nuclear materials, 2008

### OUTREACH

- **M. Stan**, *Science, Cinema and Society*, Illinois Institute of Technology, Sept. 19, 2018.
- **M. Stan**, participation in literary panel, Harold Washington Library, Chicago, Sept. 11, 2018: <https://chpublib.bibliocommons.com/events/5b48ea9145bd7b4100f3ca10>
- **M. Stan**, *Innovation: Humans and Machines*, Exelon, May 15, 2018.
- Participation in *Work/life balance*, panel discussion organized by the Next Generation Society, ANL, May 3, 2018.
- **M. Stan**, *Science, Cinema and Society*, Summer Students Seminar, ANL, June 27, 2018.
- Discussion with the Launchpad Program Cohort 2, ANL, Dec. 2017.
- **M. Stan**, *Romania*, Argonne Hispanic and Latino Club, ANL, Dec. 5, 2017.

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- **M. Stan**, *How to Get a Job after a Postdoctoral Appointment: Lessons from Soccer*, Argonne Postdoctoral Symposium, ANL, Nov. 2, 2017

### MEDIA COVERAGE

- *Argonne National Laboratory*: [The new science-machine partnerships, Argonne aims to be at the forefront of artificial intelligence research.](#)
- [Marius Stan, The Case for Artificial Intelligence](#)
- [Marius Stan, Adapting to Artificial Intelligence](#)
- [Marius Stan, Partnering with Artificial Intelligence](#)
- [Marius Stan, The Evolution of Artificial Intelligence](#)
- [Marius Stan, Advancing Artificial Intelligence](#)
- *Chicago Tribune*: [Is Stranger Things real? Argonne scientist says yes, sort of](#)
- *Argonne Today*: [ATPESC: "Computational Science and Cinema"](#)
- *University of Chicago News*: ['Breaking Bad' actor/Argonne scientist Marius Stan dishes on similarities between science and cinema](#)
- *Daily Herald*: [Argonne scientist moonlights as 'Breaking Bad' actor](#)
- *Reddit*: [I am Marius Stan, a senior scientist at Argonne](#)
- *Ziare.com*: [Consilier stiintific in guvernul SUA convins ca poate sa schimbe lumea in bine](#)

### OTHER AREAS OF INTEREST

- Philosophy of Science: focus on epistemology and the scientific method.
- Literature: received the "Orizont" award at the "Marin Preda" national contest for short stories (1988). Published a book of short stories titled "A few days" (in Romanian, 2013) and a book of poetry titled "A living fire" (in Romanian, 2015).
- Acting in movies and TV series (*Breaking Bad* and *Crash*).
- Fluent in English, Romanian, and French; good knowledge of Italian and Spanish.

### PATENTS

- 1) A. M. Yacout, M. J. Pellin, and **M. Stan**, *Designed Porosity Materials in Nuclear Reactor Components*, Patent number: US9437335B2 (2016).
- 2) S. G. Srivilliputur, M. I. Baskes, **M. Stan**, and F. J. Cherne, *A Low Temperature Method for Cleaving and/or Producing Thin Films of Solid Material*, Patent pending.

### PEER-REVIEWED PUBLICATIONS (selection enclosed)

1 book, 9 book chapters, 87 journal articles, 11 scientific reports, 228 presentations (28 keynote, 103 invited), 1,693 citations, h-index 25, i10-index 42.

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### PEER-REVIEWED PUBLICATIONS (selection, in English)

1 book, 9 book chapters, 87 journal articles, 11 scientific reports, 228 presentations (28 keynote, 103 invited), 1,570 citations, h-index 23, i10 index 40.

### Books

- 1) **M. Stan**, “Models and Simulations,” Taylor and Francis (2022).

### Book Chapters and Reports

- 1) **M. Stan**, *Physics-Based Models Across Multiple Scales*, in Transformative Manufacturing Factual Document (2020).
- 2) P. Beckman, ..., **M. Stan et al.**, *5G-Enabled Energy Innovation*, Advanced Wireless Networks Workshop for Science Report, P. Beckman (Ed), 2020, DOI:10.2172/1606538.
- 3) **M. Stan** and J. L. Sarrao, *Mesoscale Challenges: Modeling Microstructure Evolution*, in “Handbook of Materials Modeling,” 2<sup>nd</sup> Edition, Springer (2018).
- 4) L. Malerba, T. Besmann, **M. Stan et al.**, “State-of-the-Art Report on Structural Materials Modelling,” Nuclear Science NEA/NSC/R/ (2016).
- 5) C. Valot, M. Bertolus, L. Malerba, J. Rachid, T. Besmann, R. Masson, S. Phillpot, and **M. Stan**, *Integrated Multi-scale Modelling and Simulation of Nuclear Fuels*, in “State-of-the-Art Report on Multi-scale Modelling of Nuclear Fuels,” Nuclear Science NEA/NSC/R/(2015)5, September 2015.
- 6) **M. Stan**, *Coupling Methods for Multi-Scale Models and Simulations*, in “Multi-Scale Modeling Methods,” Edited by the Nuclear Energy Agency, (2015).
- 7) **M. Stan**, *Introduction to Computation*, in “Characterization of Materials,” E. Kaufman (Ed), J. Wiley & Sons, 2nd Edition, (2012) pp 115-119.
- 8) **M. Stan**, *Multi-Scale Computational Characterization*, in “Characterization of Materials,” E. Kaufman (Ed), J. Wiley & Sons, 2nd Edition (2012) pp. 174-183.
- 9) **M. Stan** and S. R. Lee, *High Performance Computing for Materials Science*, in “Handbook of Nuclear Engineering,” D. G. Cacuci (Ed.), Springer, New York (2010) pp.1499-1512.

### Journal articles

#### A) Under review

- 1) **M. Stan**, N. H. Paulson, J. A. Libera, D. Dasgupta, R. Torelli, P. Pinaki, E. Jennings, and S. Som, *Real Time Optimization of Manufacturing Processes via Experiments, Physics-Based Simulations, AI/Machine Learning, and Bayesian Statistics*, npj-Comp. Mater, (2022).
- 2) L. Liang, **M. Stan**, and M. Anitescu, *Phase Transformation Kinetics in a LiFePO<sub>4</sub> Nanoparticle with Anisotropic Coherency Strains*, Chem. Phys. Let. (2022).
- 3) **M. Stan** and B. Mihaila, *The Effect of Heterogeneous Porosity on Thermal Transport in UO<sub>2</sub> Nuclear Fuels Pins*, J. Nucl. Mater. (2022).
- 4) **M. Stan**, *More Resilient Infrastructure through Materials Design*, Infrastructure Intelligence, (2022).

#### B) Published

- 1) D. Dasgupta, P. Pal, R. Torelli, S. Som, N. Paulson, J. Libera, and **M. Stan**, *Computational Fluid Dynamics Modeling and Analysis of Silica Nanoparticle Synthesis in a Flame Spray Pyrolysis Reactor*, Comb. Flame 236 (2022) 111789.
- 2) J.C. Garcia, J. Gabriel, N.H. Paulson, J. Low, **M. Stan**, and H. Iddir, *Insights from Computational Studies on the Anisotropic Volume Change of Li<sub>x</sub>NiO<sub>2</sub> at High States of Charge ( $x < 0.25$ )*, J. Phys. Chem. C, 125 (2021) 27130.
- 3) J. J. Gabriel, N. H. Paulson, T. C. Duong, C. A. Becker, F. Tavazza, U. R. Kattner and M. Stan, *Bayesian Automated Weighting of Aggregated DFT, MD, and Experimental Data for Candidate*

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- Thermodynamic Models of Aluminum with Uncertainty Quantification*, *Materialia*, 20 (2021) 101216.
- 4) J. Pan, J. Libera, N. H. Paulson and **M. Stan**, *Flame Stability Analysis of Flame Spray Pyrolysis by Artificial Intelligence*, *Int. J. Adv. Manuf. Tech.* 114 (2022) 2215.
  - 5) G. Sivaraman, L. Gallington, A. N. Krishnamoorthy, **M. Stan**, G. Csany, A. Vasquez-Mayagoitia, and C. Benmore, *Experimentally Driven Machine Learned InterAtomic Potential for a Refractory Oxide*, *Phys. Rev. Lett.* 126 (2021) 156002.
  - 6) T. C. Duong, N. H. Paulson, **M. Stan**, and S. Chaudhuri, *An Efficient Approximation of the Supercell Approach to the Calculation of the Full Phonon Spectrum*, *CALPHAD* 72 (2021) 102215.
  - 7) J. J. Low, N. H. Paulson, M. D'Mello and **M. Stan**, *Thermodynamics of Monoclinic and Tetragonal Hafnium Dioxide (HfO<sub>2</sub>) at Ambient Pressure*, *CALPHAD* 72 (2021) 102210.
  - 8) J.J Gabriel, N. H Paulson, T. C. Duong, F. Tavazza, C. Becker, S. Chaudhuri, and **M. Stan**, *Uncertainty Quantification of Atomistic (DFT and MD), Mesoscale (PFM) and Continuum (CALPHAD) Methods and the Impact on Thermodynamic Models of Metals: A Review*, *JOM* 73 (2021) 149.
  - 9) M. Levental, R. Chard, J. A. Libera, K. Chard, J. R. Elias, M. Schwarting, **M. Stan**, S. Chaudhuri, I. Foster, *Towards Online Steering of Flame Spray Pyrolysis Nanoparticle Synthesis*, *Proceedings of The International Conference for High Performance Computing, Networking, Storage, and Analysis (SC20)* (2020).
  - 10) N. H. Paulson, J. A. Libera and **M. Stan**, *Flame Spray Pyrolysis Optimization via Statistics and Machine Learning*, *Materials and Design* 196 (2020) 108972.
  - 11) G. Sivaraman, A. N. Krishnamoorthy, M. Baur, C. Holm, **M. Stan**, G. Csányi, C. Benmore, and A. Vázquez-Mayagoitia, *Machine Learning Inter-Atomic Potentials Generation Driven by Active Learning: A Case Study for Amorphous and Liquid Hafnium Dioxide*, *npj-Comp. Mater.*, 4 (2020) 104.
  - 12) N. H. Paulson, S. Zomorodpoosh, I. Roslyakova, and **M. Stan**, *Comparison of Statistically-Based Methods for Automated Weighting of Experimental Data in CALPHAD-Type Assessments*, *CALPHAD* 68 (2020) 101728.
  - 13) N. H. Paulson, B. Gould, A. Greco, and **M. Stan**, *Correlations between Temperature History and Keyhole Porosity in Selective Laser Melting*, *Additive Manufacturing*, 34 (2019) 101213.
  - 14) P. Honarmandi, N. H. Paulson R. Arroyave, and **M. Stan**, *Uncertainty of Thermodynamic Data and Phase Diagrams*, *Mod. Sim. Mater. Sc. Eng.*, 27 (2019) 034003.
  - 15) N. H. Paulson, E. Jennings, and **M. Stan**, *Bayesian Strategies for Uncertainty Quantification of the Thermodynamic Properties of Materials*, *Int. J. Eng. Sci.* 142 (2019) 74.
  - 16) N. H. Paulson, B. J. Bocklund, R. A. Otis, Z. K. Liu, and **M. Stan**, *Quantified Uncertainty in Thermodynamic Modeling for Materials Design*, *Acta Materialia*, 174 (2019) 9-15.
  - 17) L. C. Gallington, Y. Ghadar, L. B. Skinner, J. K. Richard Weber, S. V. Ushakov, A. Navrotsky, A. Vasquez-Mayagoitia, J. C. Neuefeind, **M. Stan**, J. J. Low, and C. J. Benmore, *The Structure of Liquid and Amorphous Hafnia*, *Materials*, 10 (2017) 1290.
  - 18) Y. Li, S. Y. Hu, X. Sun, and **M. Stan**, *A Review: Applications of the Phase Field Method in Predicting Microstructure and Property Evolution of Irradiated Nuclear Materials*, *npj-Comp. Mater.*, 3 (2017) 16.
  - 19) Z. G. Mei, A. M. Yacout, Y. S. Kim, G. Hofman, and **M. Stan**, *First-Principles Study of Transition-Metal Nitrides as Diffusion Barriers against Al*, *J. Nucl. Mater.*, 471 (2016) 208-13.
  - 20) M. Piro, M. J. Welland, and **M. Stan**, *On the Interpretation of Chemical Potentials Computed from Equilibrium Thermodynamic Codes*, *J. Nucl. Mater.* 464 (2015) 48-52.
  - 21) L. Liang, **M. Stan**, and M. Anitescu, *Phase-Field Modeling of Diffusion-Induced Crack Propagations in Electrochemical Systems*, *Appl. Phys. Lett.* 105, 163903 (2014) 1-5.
  - 22) Z. G. Mei, **M. Stan**, and J. Yang, *First-Principles Study of Thermophysical Properties of Uranium Dioxide*, *J. Alloys Comp.* 603, (2014) 282-286.

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- 23) D. Yun, A. M. Yacout, **M. Stan**, T. H. Bauer, A. E. Wright, *Simulation of the Impact of 3-D Porosity Distribution in Metallic U-10Zr Fuels*, J. Nucl. Mater. 448 (2014) 129-138.
- 24) A. E. Thompson, B. Merediga, **M. Stan**, and C. Wolverton, *Interatomic Potential for Accurate Phonons and Defects in UO<sub>2</sub>*, J. Nucl. Mater., 446 (2014) 155–162.
- 25) A. M. Yacout, D. Yun, **M. Stan**, and T. H. Bauer, *Simulation of the Impact of 3-d Porosity Distribution in Metallic U-10zr Fuels*, Proceedings of the ICAPP conference (2013).
- 26) Z. G. Mei and **M. Stan**, *Computational Models of Thermodynamic Properties of Uranium Nitride*, Proceedings of the Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo (2013); <http://dx.doi.org/10.1051/snamc/201401304>.
- 27) Z. G. Mei and **M. Stan**, *Pressure-Induced Phase Transitions of UN by First-Principles*, J. Alloys Comp., 588 (2013) 648-653.
- 28) D. Yun and **M. Stan**, *3-Dimensional Finite-element Analyses of Thermal Conductivity of Oxide Fuel with Spherical Porosity*, J. Mater. Res. 28 (2013) 2308-2315.
- 29) Z. G. Mei, **M. Stan**, and B. Pichler, *First-Principles Study of Structural, Elastic, Electronic, Vibrational and Thermodynamic Properties of UN*, J. Nucl. Mater, 440 (2013) 63–69.
- 30) B. Mihaila, **M. Stan**, J. Crapps, and D. Yun *Impact of Thermal Conductivity Models on the Coupling of Heat Transport, Oxygen Diffusion, and Deformation in (U,Pu)O<sub>2-x</sub> Nuclear Fuel Elements*, J. Nucl. Mater. 433 (2012) 132-142.
- 31) B. Mihaila, **M. Stan**, and J. Crapps, *Impact of Thermal Conductivity Models on the Coupling of Heat Transport and Oxygen Diffusion in UO<sub>2</sub> Nuclear Fuel Elements*, J. Nucl. Mater. 430 (2012) 221-228.
- 32) B. Mihaila, **M. Stan**, J. Crapps, D. Yun, *Simulations of Thermal and Oxygen Transport in UO<sub>2</sub> Fuels: Impact of Thermal Conductivity*, Trans. Am. Nucl. Soc., 106 (2012) 1238-1239.
- 33) **M. Stan** and B. Mihaila *Simulations of Thermal and Oxygen Transport in UO<sub>2</sub> Fuels*, Trans. Am. Nucl. Soc., 104 (2011) 279-280.
- 34) D. Yun, G.L. Hofman, Y.S. Kim, A.M. Yacout, **M. Stan**, *Finite Element Modeling of Irradiation Induced Swelling and Creep in Metallic Mini-Plate Fuel - A Preliminary Study*, Trans. Am. Nucl. Soc., 105 (2011) 407-408.
- 35) R. Devanathan, L. Van Brutzel, A. Chartier, C. Gueneau, A. E. Mattsson, V. Tikare, T. Bartel, T. M. Besmann, **M. Stan**, and P. Van Uffelen, *Modeling and Simulation of Nuclear Fuel Materials*, Energy Environ. Sci. 3 (2010) 1406-1426.
- 36) T.M. Besmann, R.E. Stoller, G. Samolyuk, P.C. Schuck, J.M. Wills, **M. Stan**, B.D. Wirth, S. Kim, D.D. Morgan, I. Szlufarska, *Modeling Deep Burn Particulate Nuclear Fuel*, Trans. Am. Nucl. Soc., 102 (2010) 749-750.
- 37) **M. Stan**, *Discovery and Design of Nuclear Fuels*, Materials Today 12 (2009) 20-28.
- 38) B. Mihaila, **M. Stan**, J. C. Ramirez, A. Zubelewicz, and P. Cristea, *Simulations of Coupled Heat Transport, Oxygen Diffusion, and Thermal Expansion in UO<sub>2</sub> Nuclear Fuel Elements*, J. Nucl. Mater. 394 (2009) 182-189.
- 39) S. Hu, C.H. Henager Jr, H.L. Heinisch, **M. Stan**, M.I. Baskes, S.M. Valone, *Phase-Field Modeling of Gas Bubbles and Thermal Conductivity Evolution in Nuclear Fuels*, J. Nucl. Mater. 392 (2009) 292–300.
- 40) **M. Stan**, *Multi-Scale Models and Simulations of Nuclear Fuels*, J. Nucl. Eng. Technology, 41 (2009) 39-52.
- 41) **M. Stan** and S. Yip, *Design and Evaluation of Nuclear Fuels and Structural Materials: Predictive Modeling and High-Performance Simulations*, white paper for the Joint Office of Science and Office of Nuclear Energy Workshop on Advanced Modeling and Simulation for Nuclear Fission Energy Systems, Washington DC, May 11-2, 2009, available at: <https://www.cels.anl.gov/events/workshops/extremecomputing/nuclearenergy/agenda.php>.
- 42) **M. Stan**, *Innovative Nuclear Fuels: Results and Strategy*, Proceedings of the Top Fuel 2009 Conference, Paris, France, Sept. 6-10, 2009, paper 2143.

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- 43) **M. Stan**, *Theory-Based Models and Simulations of Materials for Fusion*, white paper (2009), available at:  
[http://burningplasma.org/web/renew\\_whitepapers\\_theme4.html](http://burningplasma.org/web/renew_whitepapers_theme4.html).
- 44) S. S. Hecker and **M. Stan**, *Plutonium Metallic Fuels for Fast Reactors*, J. Nucl. Mater. 383 (2008) 112–118.
- 45) **M. Stan**, J. C. Ramirez, P. Cristea, S. Y. Hu, C. Deo, B. P. Uberuaga, S. Srivilliputhur, S. P. Rudin, and J. M. Wills, *Models and Simulations of Nuclear Fuel Materials Properties*, J. Alloys Comp., 444–445 (2007) 415–423.
- 46) S. Y. Hu, M. I. Baskes, **M. Stan** and J. N. Mitchell, *Phase-Field Modeling of Coring Structure Evolution in Pu-Ga Alloys*, Acta Mater., 55 (2007) 3641-3648.
- 47) S. Y. Hu, M. I. Baskes, **M. Stan** and C. Tome, *Phase-Field Modeling of Micro-void Evolution under Elastic-plastic Deformation*, Appl. Phys. Lett., 90 (2007) 81921-81923.
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### Scientific Reports

- 1) **M. Stan**, “*The Thermodynamics and Kinetics of Truchas*”, Los Alamos National Laboratory Report, LA-UR-00-5749, 2000.
- 2) E. J. Luckwald and **M. Stan**, “*Modeling the Excess Gibbs Free Energy of an Mg-Li Liquid Solution*”, Los Alamos National Laboratory Report, LA-UR-00-4709, 1999.
- 3) D. G. Kolman, Y. Park, **M. Stan**, R. J. Hanrahan Jr., and D. P. Butt, “*An assessment of the Validity of Cerium Oxide as a Surrogate for Plutonium Oxide Gallium Removal Studies*,” Los Alamos National Laboratory Report, LA-UR-99-491, 1999.
- 4) D. P. Butt and **M. Stan**, “*On the Maximum Acceptable Gallium Concentration in MOX Fuel: A Thought Exercise*,” Los Alamos National Laboratory Report, LA-UR-98-2854, 1998.
- 5) R. J. Hanrahan, S. L. Eaton, D. P. Butt, **M. Stan**, C. L. Haertling, and Y. Park, “*Nuclear Fuels Technologies Fiscal Year 1998 Fuel Fabrication Development Gallium Sintering Summary Report*”, Los Alamos National Laboratory Report, LA-UR-98-4932, 1998.
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- 7) D. P. Butt, R. J. Hanrahan, Jr., Y. Park, and **M. Stan**, “*Thermodynamics, Phase Relationships, and the Kinetics of Gallium Removal from Mixed Oxide Fuel Fabricated with Weapons Grade Plutonium*,” Los Alamos National Laboratory Report, LA-UR-97-4719, 1997.
- 8) D. P. Butt, R. J. Hanrahan, Jr., Y. Park, **M. Stan**, and T. C. Wallace, Sr., “*Thermodynamics and Kinetics of Ga in MOX*,” Los Alamos National Laboratory Report, LA-UR-97-3853, 1997.
- 9) D. P. Butt, **M. Stan**, and D.G. Kolman, “*Ga Issues in 3013 Containers*”, Los Alamos National Laboratory Report, LA-UR-97-2866, 1997.
- 10) **M. Stan**, “*A Model for the Composition Modifications in the Cu-Sb-O System*”, Los Alamos National Laboratory Report, LA-UR-97-2020, 1997.
- 11) H. R. Trelue, T. Baros, H.T. Blair, J. J. Buksa, D. P. Butt, K. Chidester, S. F. DeMuth, S. L. Eaton, G. L. Havrilla, R. J. Hanrahan, Jr., C. A. James, D. G. Kolman, R. E. Mason, Y. Park, **M. Stan**, J. H. Steele, Jr., S. S. Vos, T. C. Wallace, Sr., C. G. Worley, “*Nuclear Fuels Technologies Fiscal Year 1997 Research and Development Test Results*”, Los Alamos National Laboratory Report, LA-UR-97-4423, 1997.

### Seminars and Conference Presentations

- 1) **M. Stan**, N. Paulson, J. Libera, D. Dasgupta, J. Gabriel, T. Duong, J Low, J. Iten, A. Clarke and C. Johnson, *Intelligent Material and Process Design*, Manufacturing Day, Online, Oct. 2, 2020 (invited).

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- 2) **M. Stan**, B. Gulsoy and P. Voorhees, *First UQPET Workshop*, UQPET Workshop (online), September 24 and 29, 2020.
- 3) **M. Stan**, Understanding Materials: Humans and Machines, MateriAIZ Seminar Series, University of Arizona (online), Sept. 18, 2020 (invited).
- 4) J. J. Gabriel, J. Garcia, N. H. Paulson, J. J. Low, **M. Stan**, and H. Iddir, Machine Learning Force Fields for Li-Ion Cathodes, NIST Atomistic Simulations for Industrial Needs (online) August 5, 2020.
- 5) **M. Stan**, N. H. Paulson, C. Niu, P. Voorhees, G. B. Olson, U. Kattner and C. Campbell, *Uncertainty Quantification of Phase Equilibria and Thermodynamics (UQPET) Tool Group*, CHiMaD Annual Meeting, Northwestern University (online), June 9, 2020 (invited)
- 6) Noah H. Paulson, J. Libera and **M. Stan**, *Machine Learning Exploration and Optimization of Flame Spray Pyrolysis*, TMS Annual Meeting, San Diego, CA, February 23-27, 2020.
- 7) **M. Stan**, Noah H. Paulson, and J. Libera, *Artificial Intelligence for Material and Process Design*, TMS Annual Meeting, San Diego, CA, February 23-27, 2020.
- 8) **M. Stan**, *The Changing Role of Computation in Material and Process Design*, NuFuel-MMSNF Workshop, Paul Scherrer Institute, Zurich, Switzerland, Nov. 4-7, 2019 (keynote, invited).
- 9) **M. Stan**, *Intelligent Material and Process Design*, 4th International Symposium of Quantum Beam Science, Ibaraki University, Hitachi, Japan, Oct. 31-Nov.2, 2019 (keynote, invited).
- 10) **M. Stan**, *Artificial Intelligence for Material and Process Design*, Tribology Frontiers Conference (TFC) Chicago, Oct. 22, 2019 (keynote, invited).
- 11) N.H. Paulson, B. Bocklund, R. Otis, **M. Stan**, and Z.-K. Liu, *PDUQ – Phase Diagram Uncertainty Quantification in Python*, 2019 Materials Science and Technology Technical Meeting and Exhibition, Portland, OR, Oct. 3, 2019.
- 12) **M. Stan**, *How to Get a Job after the Postdoctoral Appointment: Lessons from Sports*, Argonne Postdoctoral Symposium, ANL, September 18, 2019 (invited).
- 13) **M. Stan**, *Artificial Intelligence and the Scientific Method*, PSE-AI for Science and Engineering town hall, Argonne, August 1, 2019.
- 14) **M. Stan**, *Intelligent Material and Process Design*, CHiMaD Materials Design & Data Informatics Workshop, Northwestern University, July 26, 2019 (invited).
- 15) **M. Stan**, *Artificial Intelligence for Material and Process Design*, EGS Student Seminar Argonne, July 18, 2019.
- 16) **M. Stan**, *Artificial Intelligence for Material and Process Design*, PSE-AI for Science and Engineering town hall, Argonne, July 11, 2019.
- 17) **M. Stan**, *Science and Cinema*, Smithsonian Institute, June 25, 2019 (invited).
- 18) **M. Stan**, *Science and Cinema*, Global Voices Performing Arts & Lecture Series, University of Chicago, June 8, 2019 (invited).
- 19) **M. Stan**, *Science and Cinema*, DOE Triennial Review of the Center for Nanoscale Materials, June 4, 2019 (invited).
- 20) **M. Stan**, *Intelligent Material and Process Design*, Applied Materials Division Seminar Argonne, May 2, 2019.
- 21) **M. Stan**, *Artificial Intelligence for Modeling and Optimization of Complex Systems*, CEEESA seminar, Argonne, April 26, 2019 (invited).
- 22) **M. Stan**, *Phase Field Simulations of Porosity Evolution*, Illinois Institute of Technology April 22, 2019 (Invited).
- 23) **M. Stan**, *Near Real-Time Optimization of Manufacturing Processes via Machine Learning*, MSEI Workshop, Argonne, April 17, 2019.
- 24) N. H. Paulson and **M. Stan**, *Enhancing Thermodynamic Property Models and Phase, Stability Predictions through Bayesian Statistics*, University of Illinois at Chicago, Civil and Materials Engineering, Chicago, IL, April 5, 2019.
- 25) **M. Stan** and N. H. Paulson, *Uncertainty Quantification of Thermodynamic Models and Phase Diagrams*, 35th SRG Annual Meeting, Northwestern University, 25-26 March 2019 (invited).

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- 26) **M. Stan** and N. H. Paulson, *Toward Equilibrium*, TMS Annual Meeting & Exhibition San Antonio, TX, March 10-14, 2019 (invited).
- 27) N. H. Paulson, B. J. Bocklund, R. A. Otis, Z. K. Liu, and **M. Stan**, *Evaluation and Representation of Uncertainty in Thermodynamic Phase Diagrams*, TMS Annual Meeting & Exhibition, San Antonio, TX, March 10-14, 2019.
- 28) N. H. Paulson, E. Jennings, and **M. Stan**, *Bayesian Model Selection, Calibration and Uncertainty Quantification of Thermodynamic Properties*, 2019 SIAM conference on Computational Science and Engineering, Spokane, WA, February 25-March 3, 2019.
- 29) N. H. Paulson and **M. Stan**, *Bayesian fundamentals - Model Calibration and Selection*, Methods Series - National Institute for Standards and Technology, Gaithersburg, MD, February 12, 2019.
- 30) **M. Stan**, N. H. Paulson and E. Jennings, *Improved Thermodynamic Models of Complex Materials*, Big Data Challenges for Predictive Modeling of Complex Systems Conference, Hong Kong, Nov. 26-30, 2018 (keynote).
- 31) N. H. Paulson, E. Jennings, and **M. Stan**, *Bayesian Model Selection, Calibration and Uncertainty Quantification of Thermodynamic Properties*, 2019 SIAM Conference on Computational Science and Engineering, Spokane, WA, February 25-March 3, 2019.
- 32) N. H. Paulson, E. Jennings, and **M. Stan**, *A Bayesian Framework for Calibration and Uncertainty Quantification of Thermodynamic Property Models*, MRS Conference, Boston, MA, Nov. 25-30, 2018.
- 33) **M. Stan**, *Intelligent Materials Design*, Seminar, Pennsylvania State University, Oct. 11, 2018 (invited).
- 34) J. Low, **M. Stan**, J. Sun, J. W. Furness, and J. T. Russel, *Ab-Initio Molecular Dynamics (AIMD) of Urania without Metastable States*, Seattle, WA, 4–18 October 2018.
- 35) N. H. Paulson, E. Jennings and **M. Stan**, *Bayesian Analysis of Thermodynamic Data*, SIAM Conference on Mathematical Aspects of Materials Science, Portland, OR, July 9-13, 2018.
- 36) N. H. Paulson, E. Jennings and **M. Stan**, *A Bayesian Framework for the Development of Thermodynamic Property Models with Quantified Uncertainty*, 47th CALPHAD International Conference, Juriquilla Mexico, May 27-June 1, 2018 (invited).
- 37) N. H. Paulson, N. B. Gould, A. Yanguas-Gil, M. De La Cinta Lorenzo Martin, D. Singh, A. Greco and **M. Stan**, *Reduced-Order Modeling of Selective Laser Sintering*, Additive Manufacturing Conference, Argonne, May 22-24, 2018.
- 38) **M. Stan**, *Future Knowledge: Humans and Machines*, Future Compute: A celebration of the Computation Institute, University of Chicago, May 16, 2018 (invited).
- 39) **M. Stan**, *Computational Science, Art, and Society*, 30th International Conference on Parallel Computational Fluid Dynamics, Parallel CFD2018, Indianapolis, IN, May 16, 2018 (keynote).
- 40) N. H. Paulson, E. Jennings and **M. Stan**, *The Development of the Thermodynamic Property Models with Quantified Uncertainty*, seminar at the National Institute of Standards and Technology (NIST), May 10, 2018.
- 41) **M. Stan**, *Computational Materials Science: Humans and Machines*, Seminar, Notre Dame University, May 4, 2018 (keynote).
- 42) **M. Stan** and N. H. Paulson, *Uncertainty of Thermodynamic Data for Materials Design*, TMS Annual Meeting & Exhibition, Phoenix, AZ, March 11-15, 2018 (invited).
- 43) **M. Stan**, *Computational Thermodynamics: Humans and Machines*, TMS Annual Meeting & Exhibition, Phoenix, AZ, March 11-15, 2018 (invited).
- 44) Y. Ghadar, L. Gallington, L. Skinner, J.K. Weber, Sergey V. Ushakov, A. Novrotsky, A. Vazquez Mayagoitia, and **M. Stan**, *Determining the Structural Properties of Hafnia Utilizing Reactive Force Fields*, American Physical Society March Meeting, Los Angeles, CA, March 5-9, 2018.
- 45) **M. Stan**, *Artificial Intelligence: The Human-Machine Partnership*, Artificial Intelligence: The Human-Machine Partnership workshop, Argonne, Nov. 29, 2017.
- 46) **M. Stan**, *Quality of Material Property Models*, Materials Science and Technology (MS&T) Conference, Pittsburgh, PA, Oct. 9-12, 2017 (invited)

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- 47) **M. Stan**, *Uncertainty of Thermodynamic Data: Humans and Machines*, MMSNF Conference, Gatineau, Canada, Oct. 3-4, 2017 (keynote).
- 48) **M. Stan** and N. Paulson, *Uncertainty of Thermodynamics Data*, Materials Research & Data Science Conference, Rockville, MD, Sept. 25-27, 2017 (invited).
- 49) **M. Stan** and J. Warren, *The Intersection between Material Genome Initiative and Artificial Intelligence*, Materials Research & Data Science Conference, Rockville, MD, Sept. 25-27, 2017 (keynote).
- 50) **M. Stan**, *From Atoms to Material: Humans and Machines*, C-ESC Workshop, University of Cambridge, UK, Sept. 8-20, 2017 (invited).
- 51) **M. Stan**, *Reduced-Order Modeling for Additive Manufacturing*, the Additive Manufacturing Workshop, Argonne, IL USA, August 28, 2017 (invited).
- 52) **M. Stan**, *Uncertainty of Thermodynamic Properties: Humans and Machines*, ATPESC meeting, St. Charles, IL, Aug. 5, 2017 (keynote).
- 53) **M. Stan**, L. Li, and S. Y. Hu, *Phase Field simulations of Irradiation Effects*, CHiMaD Phase Field Methods 5<sup>th</sup> Workshop, Northwestern University, Aug. 1-3, 2017 (invited).
- 54) **M. Stan**, *Non-Equilibrium Thermodynamics of Multi-Component Systems*, Complex Physical Systems Workshop, ANL, Jun. 22, 2017.
- 55) **M. Stan**, *Uncertainty of Thermodynamic Data: Humans and Machines*, Machine Learning at Argonne National Laboratory Workshop, March 14-15, 2017.
- 56) **M. Stan**, *Uncertainty of Phase Diagrams via Machine Learning*, the 9th International Conference on Advanced Materials ROCAM 2017, July 5-10, 2017 (invited).
- 57) **M. Stan**, *Science, Business, and Society*, International Conference on Business Excellence, Bucharest, Romania, March 30, 2017 (keynote).
- 58) **M. Stan**, *Physics, Art, and Society*, University of Bucharest, Faculty of Physics, Bucharest, Romania, March 29, 2017 (invited).
- 59) **M. Stan**, *Science, Art and Education*, Academy of Economic Sciences, Bucharest, Romania, March 28, 2017 (invited).
- 60) **M. Stan**, *Chemistry, Art, and Society*, "Ilie Murgulescu" Institute of Physical Chemistry, Bucharest, Romania, March 28, 2017 (invited).
- 61) **M. Stan**, *Science, Art and Society*, Romanian Academy, Bucharest, Romania, March 27, 2017 (keynote).
- 62) **M. Stan**, *Certainty and Uncertainty at Multiple Scales*, Quantification of Uncertainty in Materials Science Workshop, Gaithersburg, MD, Jan. 14, 2017 (invited).
- 63) **M. Stan**, *Certainty and Uncertainty at High Temperatures*, Structure and Thermodynamics of Oxides at High Temperature (STOHT16) Conference, Univ. of California, Davis, Oct. 21-22, 2016 (invited).
- 64) **M. Stan**, *Certainty and Uncertainty at Multiple Scales*, Quantification of Uncertainty in Materials Science Workshop, Gaithersburg, MD, Jan. 14, 2016 (invited).
- 65) **M. Stan**, *Bridging Scales in Modeling and Experimentation*, The Modeling and Experimental Validation Summer School, ORNL, Aug. 20, 2016 (invited).
- 66) **M. Stan** and P. Cristea, *Certainty and Uncertainty of Thermodynamic Data*, RomPhysChem 16 Conference, Galati, Romania, Sept. 21-24, 2016 (invited).
- 67) **M. Stan**, *Materials Design for Energy Applications*, Seminar at Northwestern University, Feb. 25, 2016 (invited).
- 68) **M. Stan**, *Computational Science for Energy Applications*, Lecture at South Florida University, March 1, 2016 (invited).
- 69) **M. Stan**, Z. G. Mei, A. D. R. Andersson, J. J. Low, A. Thompson, A. Lopez Bezanilla, C. R. Stanek, C. M. Wolverton, and P. B. Littlewood, *Chemical and Heat Transport in Uranium Oxide*, CERAMICS 2015 Conference, Chicago, IL, August 17-18, 2015 (invited).
- 70) **M. Stan**, *Materials Design for Energy Applications*, ROCAM Conference, Bucharest, Romania, July 5-10, 2015 (keynote).

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- 71) L. Liang, **M. Stan**, and M. Anitescu, *Phase Field Modeling of The Li<sub>2</sub>O<sub>2</sub> Growth in a Porous Cathode in Li-Air Batteries with Organic Electrolytes*, 227<sup>th</sup> Electrochemical Society Meeting, Chicago, May 24-28, 2015.
- 72) **M. Stan**, *Nuclear Energy Advanced Modeling and Simulation (NEAMS)*, WPMM Meeting, Paris, France, May 5-7, 2015 (keynote).
- 73) **M. Stan**, *Science and Cinema*, NURETH-16, Chicago, IL, Sept. 2, 2015 (keynote).
- 74) **M. Stan**, *Computational Science and Cinema*, ATPESC, St. Charles, IL, Aug. 13, 2015 (invited).
- 75) **M. Stan**, *Science and Cinema*, MeV Summer School, Argonne National Laboratory, July 29, 2015 (invited).
- 76) **M. Stan**, *Modeling and Simulation Coordination at DOE Office of Nuclear Energy*, ANS Annual Meeting, Reno, NV, June 16-20, 2014 (invited).
- 77) Z. G. Mei, **M. Stan**, A. M. Yacout, and J. Yang, *Atomistic Study of the Effects of Point Defects and Xe Atoms on the Thermal Conductivity of UO<sub>2</sub>*, TMS Meeting, San Diego, CA, Feb. 16-20, 2014.
- 78) **M. Stan** and Z. G. Mei, *EAM insight into the phase stability of alloys*, TMS Meeting, San Diego, CA, Feb. 16-20, 2014 (invited).
- 79) Z. G. Mei and **M. Stan**, *Computational Models of Thermodynamic Properties of Uranium Nitride*, SNA+MC 2013, Paris, France, Oct. 27-31, 2013.
- 80) Z. G. Mei and **M. Stan**, *First-principles study of phase stability and thermodynamic properties of uranium nitride*, Materials Science & Technology 2013, Montreal, Quebec, Canada, Oct. 27-31, 2013.
- 81) Z. G. Mei and **M. Stan**, *Thermodynamics and Phase Stability of UN by DFT*, MMSNF 2013, Chicago, IL, Oct. 14-16, 2013.
- 82) **M. Stan**, Z. G. Mei, A. E. Thompson and C. M. Wolverton, *Thermodynamic Models of UO<sub>2</sub> and UN*, MMSNF 2013, Chicago, IL, Oct. 14-16, 2013 (invited).
- 83) **M. Stan**, Z. G. Mei, A. E. Thompson, and C. M. Wolverton, *Computational Thermochemistry of Uranium Dioxide and Uranium Nitride*, Romanian Conference of Physical Chemistry, Bucharest, Romania, Sept. 11-13, 2013 (keynote).
- 84) **M. Stan**, *Microstructural Heterogeneity and Thermal Transport*, PRICM-8 Conference, Waikoloa, HI, Aug. 4-9, 2013 (invited).
- 85) A. M. Yacout, D. Yun, and **M. Stan**, *Simulation of the Impact of 3-D Porosity Distributions on Thermal Transport in Metallic U-10Zr Fuels*, ICAPP Conference, Jeju Island, Korea, April 14-18, 2013.
- 86) **M. Stan**, B. Mihaila, D. Yung, Z. G. Mei, and P. Cristea, *Heterogeneity Effects on the Thermal Conductivity of UO<sub>2+x</sub>*, TMS Meeting, San Antonio, TX, March 3-7, 2013 (invited).
- 87) Z. G. Mei, **M. Stan**, P. Cristea, and A. D. Andersson, *Defect and Diffusion in UO<sub>2+x</sub> by Quantum Mechanics and Statistical Thermodynamic Approaches*, TMS Meeting, San Antonio, TX, March 3-7, 2013.
- 88) **M. Stan**, *Controlled Heterogeneity of Reactor Materials*, NuMat 2012 Conference, Osaka, Japan, Oct 22-26, 2012 (keynote).
- 89) **M. Stan**, *Multi-Scale Heat Transport and Chemical Diffusion*, MS&T Conference, Pittsburgh, PA, Oct. 8-12, 2012 (invited).
- 90) **M. Stan** and P. Cristea, *Computer Simulations of Materials under Extreme Conditions: Application to Nuclear Reactor Materials*, ROCAM Conference, Brasov, Romania, Aug. 28-31, 2012 (keynote)
- 91) P. Cristea, **M. Stan**, and Z. G. Mei, *Thermodynamic and Kinetic Properties of Non-Stoichiometric Nuclear Fuels*, ROCAM Conference, Brasov, Romania, Aug. 28-31, 2012 (invited).
- 92) **M. Stan**, B. Mihaila, J. Crapps, and D. Yun, *Thermal and Oxygen Transport in UO<sub>2</sub> Fuel Elements*, ANS Meeting, Chicago, IL, June 24-28, 2012.
- 93) **M. Stan**, *Multi-Scale Simulation Methods for Nuclear*, Multi-Scale Simulations of Nuclear Materials - Workshop, ANL, June 4, 2012.
- 94) **M. Stan**, *Phase Field Method Simulations of Microstructure Evolution*, Multi-Scale Simulations of Nuclear Materials - Workshop, ANL, June 4, 2012.

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- 95) **M. Stan**, *Computational Microscopy*, Univ. of California Santa Barbara Seminar, Goleta, CA, April 16, 2012 (keynote).
- 96) **M. Stan**, *Heterogeneity of Nuclear Fuels*, MRS Spring Meeting, San Francisco, CA, April 9-13, 2012.
- 97) **M. Stan**, *Bridging the Micro and Macro Scales*, MIT Seminar, March 20, 2012 (invited).
- 98) **M. Stan**, *Heterogeneity of Nuclear Fuels*, Materials Modeling and Simulation for Nuclear Fuels (MMSNF) workshop, Aix en Provence, France, Sept. 26-28, 2011.
- 99) Di Yun, A. M. Yacout, G. L. Hofman, Y. S. Kim, and **M. Stan**, *Finite Element Modeling of Irradiation Induced Swelling and Creep in Metallic Mini-Plate Fuel*, Materials Modeling and Simulation for Nuclear Fuels (MMSNF) workshop, Aix en Provence, France, Sept. 26-28, 2011.
- 100) **M. Stan**, *Materials Discovery and Design*, Seminar at the Illinois Institute of Technology, Chicago, March 28, 2011 (keynote).
- 101) **M. Stan**, B. Mihaila, and M. A. Bourke, *Validation of Models and Simulations of Nuclear Fuels*, TMS Annual Meeting, San Diego, CA, USA, Feb. 27 - March 3, 2011(invited).
- 102) **M. Stan** and S. Hu, *Simulations of Voids and Gas Bubbles in Irradiated Materials*, TMS Annual Meeting, San Diego, CA, USA, Feb. 27 - March 3, 2011(invited).
- 103) B. Mihaila and **M. Stan**, *Simulations of Coupled Heat Transport, Oxygen Diffusion and Thermal Expansion in  $UO_{2+x}$  Nuclear Fuel Rods*, The Nuclear Materials Conference, Karlsruhe, Germany, Oct. 4-7, 2010.
- 104) **M. Stan**, *Integration of Simulation Techniques for Nuclear Fuels*, F-BRIDGE School, JRC-ITU, Karlsruhe, Germany, Sept. 28-Oct. 2, 2010 (keynote).
- 105) **M. Stan**, *Models and Simulations of Nuclear Fuels*, CECAM-Workshop: Materials Modelling in Nuclear Energy Environments: State of the Art and Beyond, Zurich, Switzerland, April 26-29, 2010 (invited).
- 106) **M. Stan**, *Advanced Models and Simulations of Nuclear Fuels*, Materials Challenges in Alternative & Renewable Energy 2010 Conference, Cocoa Beach, FL, Feb. 21-24, 2010 (invited).
- 107) **M. Stan**, *Advanced Models and Simulations for Nuclear Energy*, Seminar, Argonne National Laboratory, Nov. 24, 2009 (invited).
- 108) **M. Stan**, *Models and Simulations of Materials: Results and Strategy*, Materials Science Seminar, Oak Ridge National Laboratory, Oct. 1, 2009 (keynote).
- 109) **M. Stan**, *Models and Simulations of Nuclear Fuels: Results and Strategy*, Materials Models and Simulations for Nuclear Fuels (MMSNF-8) Workshop, Albuquerque, NM, Oct. 19-21, 2009.
- 110) **M. Stan**, *Atomistic and Continuum Simulations of Phase Stability of Alloys - Advanced Models and Simulations of Nuclear Fuel Materials*, Characterization of Advanced Materials under Extreme Environments for the Next Generation Energy Systems Workshop, Brookhaven National Laboratory, Sept. 25-26, 2009 (invited).
- 111) **M. Stan**, *Discovery and Design of Materials*, Research Needs and Opportunities for Characterization of Activated Samples at X-Ray and Neutron User Facilities Workshop, Santa Fe, NM, Sept. 21-23, 2009 (invited).
- 112) **M. Stan**, B. Mihaila, C. F. Chen, E. P. Luther, P. Sadasivan, H. R. Trellue, and C. G. Bathke, *A Science-Based Approach to Developing Proliferation Resistant Thorium Oxide Nuclear Fuels*, Energy Security Strategy and Implementation Plan External Advisory Board Review, Los Alamos National Laboratory, Aug. 5-7, 2009.
- 113) **M. Stan**, *Models and Simulations for Energy Applications*, The Summer Lecture Series, Los Alamos National Laboratory, June 12, 2009 (invited).
- 114) **M. Stan** and M. Defranceschi, *Raport on the Multi-scale Modelling of Fuels and Structural Materials for Nuclear Systems Working Party (WPMM)*, the OECD/NEA Nuclear Science Committee Meeting, Paris, June 10-12, 2009.
- 115) **M. Stan** and B. Mihaila, *Models and Simulations of Oxide Nuclear Fuels*, THOR Energy Meeting, Portland, OR, March 27, 2009 (invited).

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- 116) **M. Stan**, *Computer Simulations for Nuclear Energy Applications*, High Speed Computing Conference, Salishan Lodge, Gleneden Beach, OR, April 27-30, 2009 (invited).
- 117) **M. Stan**, *Models and Simulations of Irradiation Effects on Nuclear Reactor Materials*, Computational Materials Science Network (CMSN) Symposium, Univ. of Florida, Gainesville, FL, March 11-12, 2009 (invited).
- 118) **M. Stan**, *Theory-Based Models and Simulations of Materials for Fusion*, Fusion Power ReNeW Workshop, Univ. of California Los Angeles, March 2-4, 2009 (invited).
- 119) **M. Stan**, *Discovery and Design of Materials for Energy Applications*, Invited Seminar, Oak Ridge National Laboratory, Dec. 18, 2008 (invited).
- 120) **M. Stan**, *Discovery and Design of Advanced Nuclear Fuels*, Materials Research Society Fall Meeting, Boston MA, Dec. 1-5, 2008 (invited).
- 121) **M. Stan**, *Uncertainty Quantification Needs for Nuclear Energy Applications*, Information Science and Technology workshop, Los Alamos, Dec. 11, 2008 (invited).
- 122) **M. Stan**, P. Cristea, S. Y. Hu, B. Mihaila, S. M. Valone, A. D. Andersson, L. A. Morales, K. J. McClellan, and J. C. Ramirez, *Thermodynamics of Advanced Oxide Nuclear Fuels*, Materials Science and Technology Conference, Pittsburgh, PA, Oct. 5-9, 2008 (invited).
- 123) **M. Stan**, *Modeling Phase Stability of Nuclear Fuels*, Models and Simulations for Nuclear Energy workshop, Los Alamos National Laboratory, July 29-30, 2008 (invited).
- 124) **M. Stan**, *Thermodynamic Models and Simulations of Advanced Nuclear Fuels*, 5th European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2008), Venice, Italy, June 30-July 4, 2008 (keynote)
- 125) **M. Stan**, *Report on the Working Party on Multi-scale Modelling of Fuels and Structural Materials for Nuclear Systems (WPMM)*, OECD-Nuclear Energy Agency Meeting of the Nuclear Science Committee, Paris, France, June 25-26, 2008.
- 126) **M. Stan**, *The NEA/OECD Working Party on Multi-scale Modelling of Fuels and Structural Materials for Nuclear Systems (WPMM); An International Perspective on Models and Simulations*, Models and Simulations for Nuclear Energy workshop, Los Alamos National Laboratory, July 29-30, 2008.
- 127) **M. Stan**, B. Mihaila, S. M. Valone, A. D. Andersson, K. J. McClellan, L. Morales, S. D. Conradson, S. P. Rudin, J. M. Wills, P. Cristea, and J. C. Ramirez, *Models and Simulations of Advanced Oxide Fuels*, Nuclear Energy Capability Review, Los Alamos National Laboratory, May 12-16, 2008 (invited).
- 128) **M. Stan**, B. Mihaila, S. M. Valone, A. D. Andersson, K. J. McClellan, L. Morales, S. D. Conradson, S. P. Rudin, J. M. Wills, P. Cristea, and J. C. Ramirez, *Thermodynamic Models of Actinide Oxides*, Materials Capability Review, Los Alamos National Laboratory, April 28 – May 1, 2008 (invited).
- 129) **M. Stan**, C. Tome, R. A. Lebensohn, M. I. Baskes, S. Y. Hu, C. H. Henager, *Models of Radiation Effects in Nuclear Fuels and Material*, Materials Capability Review, Los Alamos National Laboratory, April 28 – May 1, 2008 (invited).
- 130) **M. Stan**, *Thermodynamics of Nuclear Fuel Materials*, MRS Spring Conference, San Francisco, CA, March 24-28, 2008 (invited).
- 131) P. Cristea and **M. Stan**, *Analytical Model of Defect Configurational Entropy of  $\text{PuO}_{2-x}$  And  $\text{CeO}_{2-x}$* , MRS Spring Conference, San Francisco, CA, March 24-28, 2008.
- 132) **M. Stan**, *The NEA/OECD Working Party on Multi-scale Modelling of Fuels and Structural Materials for Nuclear Systems (WPMM)*, Transmutation Fuel Integration Group meeting, Salt Lake City, UT, Feb. 12-14, 2008 (invited).
- 133) **M. Stan**, *Models and Simulations of Advanced Nuclear Fuels and Materials*, Japan Atomic Energy Agency Seminar, Tokay, Japan, Feb. 26, 2008 (keynote).
- 134) **M. Stan**, *Models and Simulations of Advanced Nuclear Fuels*, Information Seminar on Research Activities on Materials and Fuels, Univ. of Tokyo, Japan, Feb. 21, 2008 (keynote).

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- 135) **M. Stan**, *Models and Simulations of Advanced Nuclear Fuels and Materials*, OECD/NEA Working Party on Multi-Scale Modelling of Fuels and Structural Materials for Nuclear Systems, Paris, France, Jan. 15-16, 2008 (keynote).
- 136) **M. Stan**, *Models and Simulations of Advanced Nuclear Fuels*, US-Japan Models and Simulations Workgroup Meeting, Tokyo, Japan, Sept. 18-19, 2007 (keynote).
- 137) P. Cristea and **M. Stan**, *Simulations of Coupled Heat and Oxygen Diffusion in Porous Urania Fuel*, Materials Models and Simulations for Nuclear Fuels (MMSNF-6) workshop, Tokyo, Japan, Dec. 14-15, 2007.
- 138) **M. Stan**, *Models and Simulations of Advanced Nuclear Fuels*, Seminar, Oak Ridge National Laboratory, Dec. 5, 2007 (invited).
- 139) **M. Stan**, *Thermodynamics of Nuclear Fuel Materials*, MRS Conference, Boston, MA, Nov. 26-30, 2007 (invited).
- 140) **M. Stan**, *Models and Simulations of Advanced Nuclear Fuels*, Advance Fuel Cycle Conference, Nizny Novogorad, Russia, Sept 24-27, 2007 (invited).
- 141) **M. Stan**, S. Y. Hu, B. Mihaila, P. Cristea, and J. C. Ramirez, *Multiscale Simulation of Thermo-mechanical Processes in Irradiated Fission-Reactor Materials*, Computational Materials Science Network (CMSN) Symposium, Salt Lake City, UT, Sept. 13-15, 2007 (invited).
- 142) **M. Stan**, *The Scientific Method*, MSTea Seminar Series, Los Alamos National Laboratory, Los Alamos, NM, Aug. 28, 2007 (invited).
- 143) **M. Stan**, *Models and Simulations of Actinide-Based Nuclear Fuels for GNEP*, Lujan Seminar Series, Los Alamos National Laboratory, Los Alamos, NM, Aug. 7, 2007 (invited).
- 144) **M. Stan**, *Materials for Nuclear Energy*, Energy Council Meeting, Los Alamos National Laboratory, Los Alamos, NM, June 20, 2007 (invited).
- 145) S. L. Voit, K. J. McClellan, L. Morales and **M. Stan**, *Minor Actinide MOX Fuel Development for the GNEP Program*, The 8th Russian Conference on Reactor Material Science, Dimitrovgrad, Russia, May 21-25, 2007.
- 146) **M. Stan**, *Designed Materials Overview*, Materials Capability Review, Los Alamos National Laboratory, Los Alamos, NM, May 15-18, 2007 (invited).
- 147) **M. Stan**, J. C. Ramirez, P. Cristea, S. Y. Hu, C. Deo, B. P. Uberuaga, S. Srivilliputhur, S. P. Rudin, and J. M. Wills, *Models and Simulations of Nuclear Fuel Materials Properties*, Materials Capability Review, Los Alamos National Laboratory, Los Alamos, NM, May 15-18, 2007.
- 148) S. L. Voit, K. J. McClellan, L. A. Morales, **M. Stan**, *Minor Actinide MOX Fuel Development for the GNEP Program*, Materials Capability Review, Los Alamos National Laboratory, Los Alamos, NM, May 15-18, 2007.
- 149) **M. Stan** and C. R. Stanek, *Advanced Models and Simulations for Nuclear Fuels*, Transuranic Fuel Development Working Group Meeting, Salt Lake City, May 15-16, 2007 (invited).
- 150) **M. Stan**, *Thermodynamics of Nuclear materials*, I-NERI Meeting, April 26-27, 2007, Aix en Provence, France (invited).
- 151) **M. Stan**, *Models of Materials Properties for Advanced Fuel Performance Codes*, CESC Meeting, Washington D. C., April 10-12, 2007 (invited).
- 152) **M. Stan**, *Current Fuel Models and Simulations Activities at LANL*, Fuel Performance Meeting Idaho National Laboratory, March. 22-23, 2007 (invited).
- 153) **M. Stan**, *Materials for Nuclear Energy Applications*, TMS Conference, Orlando, FL, Feb. 26-March 1, 2007 (invited).
- 154) T. Watanabe, S. G. Srivilliputhur, S. B. Sinnott, J. S. Tulenko, R. W. Grimes, **M. Stan**, S. A. Maloy, and S. Phillpot, *Molecular Dynamics Simulation of Radiation Damage in Uranium Dioxide*, TMS Conference, Orlando, FL, Feb. 26-March 1, 2007.
- 155) **M. Stan**, *Advanced Fuel Performance Codes*, CEA meeting, Cadarache, France, Dec. 6, 2006 (invited).

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- 156) **M. Stan**, *Models and Simulations of Thermodynamic Properties and Transport Phenomena in  $UO_{2+x}$* , International Information Exchange Meeting on Thermodynamics of Nuclear Fuels, Saclay, Franc, Nov. 27-Dec. 1, 2006 (keynote).
- 157) S. Y. Hu, M. I. Baskes, **M. Stan** and S.G. Srivilliputhur, *Vacancy Formation Energy Near Guinier-Preston Zones and Theta' Nucleation in Al-Cu Alloys*, MSR Fall Meeting, Boston, MA, Nov. 27-Dec. 1, 2006.
- 158) S. Y. Hu, M. I. Baskes, Y. L. Li, and **M. Stan**, *Phase-field Modeling of Microstructure Evolution under Elastic-Plastic Deformation*, MSR Fall Meeting, Boston, MA, Nov. 27-Dec. 1, 2006.
- 159) **M. Stan**, *Nuclear Fuel Performance Codes Status and Requirements*, Workshop on Nuclear Fuel Performance, Washington DC, Nov. 8, 2006 (invited).
- 160) **M. Stan**, *Thermodynamics of Roses-Toward Predictive Models and Simulations*, Materials Research Seminar, Louisiana State University, Baton Rouge, LA, Oct. 27, 2006 (invited).
- 161) **M. Stan**, J.C. Ramirez, and P.Cristea, *Thermodynamics of Nuclear Fuel Materials*, High Temperature Materials Chemistry conference, HTMC, Vienna, Austria, Sept. 18-22, 2006 (invited).
- 162) **M. Stan**, *Thermodynamics of Nuclear Materials*, Romanian Conference on Advanced Materials, ROCAM 2006, Bucharest, Romania, Sept. 9-10, 2006 (keynote).
- 163) P. Cristea, **M. Stan**, and J. C. Ramirez, *Point Defects and Oxygen Diffusion in Fluorite-Type Oxides*, Romanian Conference on Advanced Materials, ROCAM 2006, Bucharest, Romania, Sept. 9-10, 2006 (invited).
- 164) **M. Stan**, *Nuclear Fuel Performance Codes Status and Requirements*, Workshop on Simulation and Modeling for Advanced Nuclear Energy Systems, Washington DC. , Aug. 15-17, 2006 (invited).
- 165) **M. Stan**, J. C. Ramirez, P. Cristea, M. I Baskes, S. M. Valone, and S.Y. Hu, *Thermodynamics of Roses-Toward Predictive Thermodynamic Models and Simulations*, THERMO International 2006 Conference, Boulder, CO, Jul. 30-Aug. 4, 2006 (invited).
- 166) **M. Stan**, *Thermodynamic and Basic Science Issues Associated with Fuels*, Workshop on Basic Research Needs for Advanced Nuclear Energy Systems, Washington DC, July 31–August 2, 2006. (invited)
- 167) **M. Stan**, B. P. Uberuaga, S. Srivilliputhur, J. C. Ramirez, C. Deo, P. Cristea, S.Y. Hu, S. P. Rudin, and J. M. Wills, *Models and Simulations of Nuclear Fuel Materials*, Pu-Futures Conference, Pacific Grove, CA, July 9-13, 2006 (invited).
- 168) S.Y. Hu, M. Baskes and **M. Stan**, *Phase-field Simulation of Coring Structure Evolution and Ga Homogenization Kinetics in Pu-Ga Alloys*, Pu-Futures Conference, Pacific Grove, CA, July 9-13, 2006.
- 169) M.I. Baskes, S.Y. Hu, S.M. Valone and **M. Stan**, *Calculated properties of PuGa Alloys using the Modified Embedded Atom Method*, Pu-Futures Conference, Pacific Grove, CA, July 9-13, 2006.
- 170) S. Y. Hu, Y. L. Li, L.Q. Chen, T. Lookman, Q. X. Jia, **M. Stan**, and M. I. Baskes, *Phase-Field Modeling of Microstructure Evolution under Elastic-Plastic Deformation*, Beijing International Materials Week (2006 BIMW), Beijing, China, June 25-30, 2006 (invited).
- 171) **M. Stan**, S. Y. Hu, and M. I. Baskes, *Multi-Scale Calculation of Thermodynamic Properties in Al-Cu Alloys*, TOFA 2006 – Discussion Meeting on Thermodynamics of Alloys, Beijing, China, June 18-23, 2006 (invited).
- 172) **M. Stan**, *Models and Simulations of Thermodynamic Properties of Nuclear Fuels*, LANL-CEA meeting, Saclay, France, June 5-9, 2006 (invited).
- 173) J. C. Ramirez, P. Cristea, and **M. Stan**, *Simulations of Heat and Oxygen Diffusion in  $UO_2$  Nuclear Fuel Rods*, MMSNF 5 workshop, Nice, France, June 1-2, 2006.
- 174) **M. Stan**, J. C. Ramirez, and P. Cristea, *Thermodynamic Models and Simulations of Nuclear Fuel Materials*, E-MRS Conference, Nice, France, May 29-June 1, 2006 (invited).
- 175) **M. Stan**, K. Muralidharan, M. I. Baskes, S. Y. Hu, and S. M. Valone, *The Entropy of Delta Phase Pu-Ga Alloys*, Enhanced Surveillance Campaign Review, Livermore, CA, April 25-27, 2006.
- 176) **M. Stan**, *Thermodynamics of Roses*, TMS 2006 135<sup>th</sup> Annual Meeting & Exhibition, San Antonio, TX, March 12-16, 2006 (invited).

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- 177) M.I. Baskes, S.Y. Hu and **M. Stan**, *Calculated Properties of Pu-Ga Alloys Using the Modified Embedded Atom Method*, TMS 2006 135<sup>th</sup> Annual Meeting & Exhibition, San Antonio, TX, March 12-16, 2006 (invited).
- 178) S.Y. Hu, M.I. Baskes, **M. Stan** and L.Q. Chen, *Molecular Dynamics Simulations of Thermodynamic Properties and Stability of Precipitates in Al-Cu Alloys*, TMS 2006 135<sup>th</sup> Annual Meeting & Exhibition, San Antonio, TX, March 12-16, 2006.
- 179) **M. Stan**, *Models and Simulations of Thermodynamic Properties of Alloys and Ceramics*, Materials Research Seminar, Colorado School of Mines, Golden, CO, Feb 2, 2006 (invited)
- 180) J.C. Ramirez, P.Cristea, S.Y. Hu, **M. Stan**, and M.I. Baskes, *Incorporating Atomistic and Phase Field Calculations into Heat, Oxygen, and Helium Transport Simulations in Nuclear Fuel Rods*, Materials Models and Simulations for Nuclear Fuels Workshop (MMSNF-4), Washington DC, Nov. 17-18, 2005.
- 181) S.Y. Hu, M. Baskes, and M.Stan, *Phase-Field Modeling of Coring Structure Evolution During bcc to fcc Transition in Pu-Ga Alloys*, LDRD DR meeting, LANL, Oct, 2005.
- 182) S.Y. Hu, M. Baskes, and M.Stan, *Phase-Field Modeling of Gas Bubble Evolution in Fuels*, "Materials Science and Technology for Nuclear Fuels" workshop on Oct. 26-27, 2005, at LANL.
- 183) **M. Stan**, *The Entropy of Delta Pu-Ga Alloys*, ANS Annual Meeting San Diego, CA, June 5-9, 2005.
- 184) **M. Stan** and B. P. Uberuaga, *Materials Models and Simulations for Nuclear Fuels*, Advanced Fuel Cycle Initiative Semi-Annual Review Meeting, Alexandria, VA, Feb. 15 - 17, 2005 (invited).
- 185) **M. Stan**, *The Entropy of Alloys*, 2005 TMS Annual Meeting & Exhibition, San Francisco, CA, Feb. 13-17, 2005.
- 186) P. Cristea and **M. Stan**, *Oxygen Diffusivity in Nonstoichiometric Cerium Dioxide*, 2005 TMS Annual Meeting & Exhibition, San Francisco, CA, Feb. 13-17, 2005.
- 187) **M. Stan**, *Prediction of Nuclear Fuel Materials Properties*, American Nuclear Society Winter Meeting, Washington DC, Nov. 14-18, 2004.
- 188) **M. Stan** and P. Cristea, *Thermochemistry of Defects and Oxygen Diffusion in PuO<sub>2-x</sub>*, American Nuclear Society Winter Meeting, Washington DC, Nov. 14-18, 2004.
- 189) **M. Stan**, *Science-Based Prediction of Nuclear Fuel Properties*, Materials Models and Simulations for Nuclear Fuels Workshop (MMSNF-3), Washington DC, Nov. 18-19, 2004.
- 190) P. Cristea, **M. Stan**, T. C. Wallace, Sr., and K. V. Woan, *Controlling Nonstoichiometry of PuO<sub>2-x</sub> and UO<sub>2+x</sub>*, Materials Models and Simulations for Nuclear Fuels Workshop (MMSNF-3), Washington DC, Nov. 18-19, 2004.
- 191) **M. Stan** and S. M. Valone, *Materials Models and Simulations for Nuclear Fuels*, Advanced Fuel Cycle Initiative Semi-Annual Review Meeting, Salt Lake City, UT, Sept. 13-15, 2004.
- 192) **M. Stan**, *The Entropy of Alloys*, TOFA 2004-Discussion Meeting on Thermodynamics of Alloys, Vienna, Austria, Sept. 12 - 17, 2004.
- 193) **M. Stan**, P. Cristea, T. C. Wallace, Sr., *Defect Thermochemistry and Phase Stability in PuO<sub>2-x</sub>*, 11th Symposium on Thermodynamics of Nuclear Materials (STNM11), Karlsruhe, Germany, Sept. 6-10, 2004.
- 194) **M. Stan**, *Phase Stability and Phase Diagrams in the Pu-Ga System*, U.S. – Russian Plutonium Science Workshop, Sarov, Russia, Aug. 30-Sept. 2, 2004.
- 195) **M. Stan**, *Thermochemistry of Defects and Oxygen Diffusion in PuO<sub>2-x</sub>*, U.S. – Russian Plutonium Science Workshop, Sarov, Russia, Aug. 30-Sept. 2, 2004.
- 196) **M. Stan**, *Models and Simulation of High Temperature Properties and Phenomena*, Gordon Research Conference on High Temperature Materials, Processes and Diagnostics, Waterville, ME, Aug. 1- 6, 2004 (invited).
- 197) **M. Stan**, S. Swaminarayan, and K. Lam, *Chemical Reaction Models in Truchas*, TRUCHAS Workshop, Los Alamos, NM, June 21-24, 2004.

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- 198) S. M. Valone, M. I. Baskes, A. C. Lawson, R. C. Mulford, S. P. Chen, R. Martin, B. P. Uberuaga, and A. F. Voter, *Atomistic Models of Radiation Damage in Plutonium*, Enhanced Surveillance Campaign Annual Review, Los Alamos, NM, March 23-25, 2004.
- 199) B. Reardon and **M. Stan**, *Model Validation Methods for Phase Diagram Determination*, SAMO-Sensitivity Analysis and Model Output Conference, Santa Fe, NM, March 8-11, 2004.
- 200) **M. Stan**, P. Cristea, and T. C. Wallace, Sr., *Phase Stability, Diffusion, and Heat Transfer in Actinide Based Ceramics and Surrogate Materials*, MMSNF2 Workshop, New Orleans, LA, Nov. 20-21, 2003.
- 201) **M. Stan**, M. I. Baskes, and K. Muralidharan, *Phase Stability in the Pu-Ga System From First Principles and Molecular Dynamics Calculations*, 2003 MRS Fall Meeting, Boston, MA, Dec. 1-5, 2003.
- 202) **M. Stan**, P. Cristea, and T. C. Wallace, Sr., *Phase Stability and Diffusion in Actinide Based Ceramics and Surrogate Materials*, Materials Models and Simulations for Nuclear Fuels Workshop (MMSNF-2), New Orleans, Nov. 18-19, 2004 (invited).
- 203) L. Popa-Simil, M. Hollander, D.R. Janecky, and **M. Stan**, *Dynamics of The Gas Production During He Ion Beam Bombardment of PTFE*, IBA-2003 Conference, Albuquerque, NM, July 1-4, 2003.
- 204) **M. Stan**, *Phase Stability and Phase Diagrams in the Pu-Ga System*, U.S. – Russian Plutonium Science Workshop, June 11, 2003, Los Alamos, NM, USA.
- 205) **M. Stan**, M. I. Baskes, S. P. Chen, and K. Muralidharan, *Phase Stability of Pu-Ga Alloys from First Principles and Molecular Dynamics Calculations*, XXXII CALPHAD Conference, La Malbay, Canada, May 25-30, 2003.
- 206) K. Muralidharan, M. I. Baskes, **M. Stan**, and S. G. Srinivasan, *Atomistic Modeling of the Phase Stability in the Pu-Ga System*, The 132nd TMS Annual Meeting & Exhibition, March 2-6, 2003, San Diego, CA, USA.
- 207) J. N. Mitchell, **M. Stan**, D. S. Schwartz, C. J. Boehlert, *Phase Transformations and Phase Stability in the Pu-Ga System*, The 132nd TMS Annual Meeting & Exhibition, March 2-6, 2003, San Diego, CA, USA.
- 208) Conference: 4th Pacific Rim International Conference on Advanced Materials and Processing (PRICM4); Honolulu, HI, Dec. 11-15, 2001.
- 209) S. M. Valone, M. I. Baskes, **M. Stan**, and K. E. Sickafus, *"Radiation Damage in Pu Metals and Alloys"*, 23<sup>rd</sup> Aging, Compatibility, and Stockpile Stewardship Conference, Livermore, CA, Nov. 14-16, 2000.
- 210) J. C. Cooley, C. J. Boehlert, D. E. Dooley, J. N. Mitchell, **M. Stan**, and D. J. Thoma, *Phase Stability in Metastable Plutonium*, 23<sup>rd</sup> Aging, Compatibility, and Stockpile Stewardship Conference, Livermore, CA, Nov. 14-16, 2000.
- 211) **M. Stan** and B. Reardon, *A Bayesian Approach to Evaluating the Uncertainty of Thermodynamic Data and Phase Diagrams*, CALPHAD XXX, York, UK, May 27 – June 1, 2001.
- 212) **M. Stan**, *The Perfect Thermodynamics of Imperfect Materials*, CALPHAD XXX, York, UK, May 27 – June 1, 2001.
- 213) **M. Stan**, M. I. Baskes, S. M. Valone, and S. P. Chen, *Predicting Thermodynamic Properties of Materials*, 2001 TMS Annual Meeting, New Orleans, LA, Feb. 11-15, 2001.
- 214) M. I. Baskes, and **M. Stan**, *An Atomistic Study of Solid-Liquid Interfaces*, 2001 TMS Annual Meeting, New Orleans, LA, Feb. 11-15, 2001.
- 215) **M. Stan**, T. Armstrong, R. J. Hanrahan, Jr., D. P. Butt, T. C. Wallace, Sr., C. L. Haertling, and Y. Park, *Study of the Stability of a Perovskite Compound in the Pu(Ce)-Ga-O System*, The 101 American Ceramic Society Conference, Indianapolis, IN, April 24-29, 1999.
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