Marius STAN, Ph.D.

Senior Computational Energy Scientist, Energy and Global Security Directorate, Argonne National Laboratory, 9700 S. Cass Ave., Argonne, IL, 60439; +1-630-252-4915; mstan@anl.gov; http://www.anl.gov/contributors/marius-stan
Senior Fellow, Computation Institute, University of Chicago, http://www.ci.uchicago.edu/profile/316
Senior Fellow, Institute for Science and Engineering, Northwestern University, http://naise.northwestern.edu/members/marius-stan

PROFILE: Computational chemist and physicist, leader of U. S. A. and international programs on modeling and simulation for energy and electronics applications.

- Pioneered the concept of "multi-scale modeling and simulation" and the associated methodology of coupling theoretical and computational methods that operate at different length and time scales, from atomistic, to meso-scale, to continuum. This methodology is now used worldwide.
- Managed U. S. A. national modeling and simulation programs of over $25 mil/year budget.
- Developed institutional, national, and international vision and strategic plans for scientific computing.

EDUCATION

- **Ph.D. (Chemistry**), Romanian Academy, Institute of Physical Chemistry, Bucharest, Romania, 1997.
- **B.S. (Physics)**, University of Bucharest, Bucharest, Romania, 1986.

PROFESSIONAL EXPERIENCE

Senior Scientist, Argonne National Laboratory (ANL), Energy and Global Security Directorate, 2010-present.

- Improves the understanding and prediction of multi-component systems properties by using elements of artificial intelligence, machine learning, and multi-scale computer simulations.
- Participates in defining goals and vision for computational chemistry, physics and materials science.
- Develops theory and models of physical systems and materials that are "heterogeneous by design".
- Improves the understanding of coupled heat transport, species diffusion, and thermal expansion of ceramics and alloys by performing Finite Element Method (FEM) simulations.
- Designs 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.
- Improves 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.

Senior Fellow, Northwestern-Argonne Institute for Science and Engineering, Northwestern Univ., 2013-present.

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

Senior Fellow, Computation Institute, University of Chicago, 2011-present.

- Improves the analysis of large data sets and data streams by using artificial intelligence and machine learning.
- Develops ZOOM, a multi-scale computational microscope.
- Prepares a course on computational science, with an emphasis on multi-scale and coupled physics.

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Senior Advisor, Department of Energy (DOE), Office of Nuclear Energy, NE-1, 2013-2015.

- 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.

National Technical Director, Department of Energy, Office of Nuclear Energy, NE-1, 2013-2015.

- 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 impact and 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).

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

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

Deputy Group Leader, LANL, Structure-Properties Relations Group, 2006-2007.

- Participated in management of group of over 100, 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.

Team Leader, LANL, Thermodynamics of Materials Team, 2005-2006.

- Created and led a computational and experimental thermodynamics of materials team of 16 staff members, postdocs and students.
- Performed advanced FEM simulations (COMSOL) of transport in nuclear fuel elements.

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

- 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_2). This methodology is now 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_2, PuO_2) that created a new 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.

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

- 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.

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

- 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.

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

- Developed mathematical models of thermodynamic properties of ceramics such as Ba(Zn)-Fe-O and Mg-Fe-O.
- Performed experimental validation using DSC, DTA, XRD, and SEM.

TEACHING EXPERIENCE

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

- 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 18 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.

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AWARDS AND HONORS

- 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".
- U. S. A. Department of Energy "Pollution Prevention Award" for innovative science and technology in nuclear materials.
- "Honorary Citizen" of the city of Urziceni, Romania.

MEDIA COVERAGE

- *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.

PEER-REVIEWED PUBLICATIONS (list enclosed)

8 books/chapters, 73 journal articles and 167 presentations (89 invited).

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PEER-REVIEWED PUBLICATIONS (selection, in English)
8 books/chapters, 73 journal articles and 167 presentations (89 invited).

Books
1) M. Stan, "Models and Simulations of Nuclear Fuels", Taylor and Francis (2017) in press.

Book Chapters
2) L. Malerba, T. Besmann, M. Stan et al., "State-of-the-Art Report on Structural Materials Modelling", Nuclear Science NEA/NSC/R/(2016), in print.
3) 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.
4) M. Stan, *Coupling Methods for Multi-Scale Models and Simulations*, in "Multi-Scale Modeling Methods", Edited by the Nuclear Energy Agency, (2015) in press.
5) M. Stan, *Introduction to Computation*, in "Characterization of Materials", E. Kaufman (Ed), J. Wiley & Sons, 2nd Edition, (2012) pp 115-119.
6) M. Stan, *Multi-Scale Computational Characterization*, in "Characterization of Materials", E. Kaufman (Ed), J. Wiley & Sons, 2nd Edition (2012) pp. 174-183.
7) 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
1) L. Liang, M. Stan, et al., *Phase-field Model for a LiO_2-Li_2O_2 Transformation in a Lithium-Air Battery*, Chem. Phys. Let. (2016) submitted.
2) L. Liang, M. Stan, and M. Anitescu, *Phase Transformation Kinetics in a LiFePO4 Nanoparticle with Anisotropic Coherency Strains*, Chem. Phys. Let. (2016) submitted.
3) M. Stan, D. Yun and B. Mihaila, *The Effect of Heterogeneous Porosity on Thermal Transport in UO_2 Nuclear Fuels Pins*, J. Nucl. Mater. (2016) submitted.
4) Y. Li, S. Y. Hu, X. Sun, and M. Stan, *A Review: Applications of the Phase Field Method in Predicting Microstructure and Property Evolution in Irradiated Materials*, Modelling Simul. Mater. Sci. Eng. (2016) accepted.
5) 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.
6) 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.
7) L. Liang, M. Stan, and M. Anitescu, *Phase-Field Modeling of Diffusion-Induced Crack Propagations in Electrochemical Systems*, Appl. Phys. Let. **105**, 163903 (2014) 1-5.
8) Z. G. Mei, M. Stan, and J. Yang, *First-Principles Study of Thermophysical Properties of Uranium Dioxide*, J. Alloys Comp. **603**, (2014) 282-286.
9) 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.
10) A. E. Thompson, B. Merediga, M. Stan, and C. Wolverton, *Interatomic Potential for Accurate Phonons and Defects in UO_2*, J. Nucl. Mater., **446** (2014) 155–162.
11) 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) accepted.
12) 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.
13) Z. G. Mei and M. Stan, *Pressure-Induced Phase Transitions of UN by First-Principles*, J. Alloys Comp., **588** (2013) 648-653.
14) 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.

15) 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.
16) 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_{2-x} Nuclear Fuel Elements*, J. Nucl. Mater. **433** (2012) 132-142.
17) B. Mihaila, M. Stan, and J. Crapps, *Impact of Thermal Conductivity Models on the Coupling of Heat Transport and Oxygen Diffusion in UO_2 Nuclear Fuel Elements*, J. Nucl. Mater. **430** (2012) 221-228.
18) B. Mihaila, M. Stan, J. Crapps, D. Yun, *Simulations of Thermal and Oxygen Transport in UO_2 Fuels*: *Impact of Thermal Conductivity*, Trans. Am. Nucl. Soc., **106** (2012) 1238-1239.
19) M. Stan and B. Mihaila *Simulations of Thermal and Oxygen Transport in UO_2 Fuels*, Trans. Am. Nucl. Soc., **104** (2011) 279-280.
20) 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.
21) 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.
22) 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.
23) M. Stan, *Discovery and Design of Nuclear Fuels*, Materials Today **12** (2009) 20-28.
24) B. Mihaila, M. Stan, J. C. Ramirez, A. Zubelewicz, and P. Cristea, *Simulations of Coupled Heat Transport, Oxygen Diffusion, and Thermal Expansion in UO_2 Nuclear Fuel Elements*, J. Nucl. Mater. **394** (2009) 182-189.
25) 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.
26) M. Stan, *Multi-Scale Models and Simulations of Nuclear Fuels*, J. Nucl. Eng. Technology, **41** (2009) 39-52.
27) 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.
28) M. Stan, *Innovative Nuclear Fuels: Results and Strategy*, Proceedings of the Top Fuel 2009 Conference, Paris, France, Sept. 6-10, 2009, paper 2143.
29) M. Stan, *Theory-Based Models and Simulations of Materials for Fusion*, white paper (2009), available at: http://burningplasma.org/web/renew_whitepapers_theme4.html.
30) S. S. Hecker and M. Stan, *Plutonium Metallic Fuels for Fast Reactors*, J. Nucl. Mater. **383** (2008) 112–118.
31) 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.
32) 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.
33) S.Y. Hu, M. I. Baskes, M. Stan and C. Tome, *Phase-Field Modeling of Micro-void Evolution under Elastic-plastic Deformation*, Appl. Phys. Let., **90** (2007) 81921-81923.
34) S. Y. Hu, M. I. Baskes, M. Stan, J. N. Mitchell, J. X. Zhang, and L. Q. Chen, *Effect of Elastic Anisotropy and Inhomogeneity on Coring Structure Evolution in Pu-Ga Alloys - Phase-field Modeling*, J. Comp.-Aided Mater. Design, **14** (2007) 389-402.
35) P. Cristea, M. Stan, and J. C. Ramirez, *Point Defects And Oxygen Diffusion in Fluorite Type Oxides*, J. Optoelectr. Advanced Mater., **9** (2007) 1750 - 1756.
36) S.Y. Hu, M. I. Baskes, M. Stan and L. Q. Chen, *MD Simulations of Interfacial Energies, Critical Nucleus Shape and Size of Plate-like Precipitates in Al-Cu Alloys*, Acta Mater., **54** (2006), 4699-4707.
37) S.Y. Hu, M. I. Baskes, M. Stan and L. Q. Chen, *Molecular Dynamic Simulations of Thermodynamic Properties and Phase Stability in Al-Cu Alloys*, TMS Letter, **3** (2006) 17-18.
38) J. C. Ramirez, M. Stan, and P. Cristea, *Simulations of Heat and Oxygen Diffusion in UO2 Nuclear Fuel Rods*, J. Nucl. Mater., **359** (2006) 174-184.

39) M. Stan, M. I. Baskes, S. M. Valone, and B. Uberuaga, Thermodynamic Properties and Radiation Damage of Delta-Pu-Ga Alloys, Materialovedenie, **9** (2005) 33-39.
40) M. Stan, M. I. Baskes, K. Muralidharan, T. A. Lee, S. Hu, and S. M. Valone, *Thermodynamic Properties of Pu-Ga Alloys*, Proceedings of the International Workshop on Fundamental Plutonium Properties, Snezhinsk, Russia, Sept. 12-16, 2005, pp. 73-75.
41) P. Cristea and M. Stan, *Oxygen Diffusivity in CeO2-x*, TMS Letters, **2** (2005) 91-92.
42) M. Stan and P. Cristea, *Thermochemistry of Defects and Oxygen Diffusion in PuO2-x*, J. Nucl. Mater, **344** (2005) 213–218.
43) M. Stan, *The Entropy of Alloys*, JOM, **56** (2004) 243.
44) P. Cristea and M. Stan, *Oxygen Diffusivity in Nonstoichiometric Cerium Dioxide*, JOM, **56** (2004) 204.
45) M. Stan, *Prediction of Nuclear Fuel Materials Properties*, T. Am. Nucl. Soc, **91** (2004) 131-133.
46) M. Stan and P. Cristea, *Thermochemistry of Defects and Oxygen Diffusion in PuO2-x*, T. Am. Nucl. Soc, **91** (2004) 491-491.
47) S. L. Voit, K. J. McClellan, and M. Stan, *Depleted Uranium Dioxide (DUO_2) Feedstock Modification and Characterization for Mixed Oxide Fuel Fabrication at the Los Alamos National Laboratory*, T. Am. Nucl. Soc, **91** (2004) 492-493.
48) M. Stan, Y. T. Zhu, H. Jiang, and D. P. Butt, *Kinetics of Oxygen Removal from Ceria*, J. Appl. Phys., **95** (2004) 3358-3361.
49) S. M. Valone, M. I. Baskes, M. Stan, T. E. Mitchell, A. C. Lawson, and K. E. Sickafus, *Simulations of Low Energy Cascades in fcc Pu Metal at 300 K and Constant Volume* J. Nucl. Mater., **324** (2004) 41-51.
50) M. Stan and B. J. Reardon, *A Bayesian Approach to Evaluating the Uncertainty of Thermodynamic Data and Phase Diagrams*, Calphad, **27** (2004) 319-323.
51) J. N. Mitchell, M. Stan, D. S. Schwartz, and C. J. Boehlert, *Phase Stability and Phase Transformations in Plutonium and Plutonium-Gallium Alloys*, Metall. Mater. Trans., **34A** (2004) 2267-2278.
52) D. G. Kolman, T. N. Taylor, Y. S. Park, M. Stan, D. P. Butt, C. J. Maggiore, J. R. Tesmer, and G. J. Havrilla, *Gallium-Induced Oxidation of Selected Pure Metals and Alloys at 1200 °C*, Proc. 205th Meeting Electrochem. Soc., (2004) 1794.
53) M. I. Baskes, K. Muralidharan, M. Stan, S. M. Valone and F. J. Cherne, *Using the Modified Embedded-Atom Method to Calculate the Properties of Pu-Ga Alloys*, JOM, **55** (2003) 41-50.
54) M. I. Baskes and M. Stan, *"An Atomistic Study of Solid/Liquid Interfaces and Phase Equilibrium in Binary Systems"*, Metal. Mater. Trans., **34A** (2003) 435-439.
55) M. I. Baskes, M. Stan, and K. Muralidharan, *"Phase Stability of Pu and Pu-Ga Alloys from Atomistic Calculations"*, AIP Conf Proc, **673** (2003) 128-130.
56) M. Stan, T. J. Armstrong, D. P. Butt, T. C. Wallace, Sr., Y. Park, C. L. Haertling, T. Hartman, and R. J. Hanrahan Jr. "*Stability of the Perovskite Compounds in the Ce-Ga-O and Pu-Ga-O Systems"* J. Amer. Ceram. Soc., **85** (2002) 2811-2816.
57) D.G. Kolman, T.N. Taylor, Y.S. Park, M. Stan, D.P. Butt, C.J. Maggiore, J.R. Tesmer, and G.J. Havrilla, *"Gallium Suboxide Attack of Stainless Steel and Nickel Alloys at 800^{o}C to 1200^{o}C"*, Oxid. Met., **55** (2001) 439-472.
58) D.G. Kolman, T.N. Taylor, Y.S. Park, M. Stan, D.P. Butt, C.J. Maggiore, J.R. Tesmer, and G.J. Havrilla *"Gallium Suboxide Vapor Attack of Chromium, Cobalt, Molybdenum, Tungsten, and Their Alloys at 1200^{o}C"*, Oxid. Met., **56** (2001) 347-374.
59) S. M. Valone, M. I. Baskes, M. Stan, and K. E. Sickafus, *Point-Defect Production and Migration in Pu Metal at Ambient Conditions*, Proceedings of the PRICM 4: Forth Pacific Rim International Conference on Advanced Materials And Processing, (2001) 2941-2943.
60) M. Stan, *Modeling the Thermodynamic Properties of Plutonium*, A. I. P. Conference Proceedings, **532** (2000) 390-391.
61) Y. T. Zhu, M. Stan, S. D. Cozone, and D. P. Butt, "*Thermal Oxidation Kinetics of $MoSi_2$-Based Powders", J*. Amer. Ceram. Soc., **82** (1999) 2785-2790.
62) M. Stan, *"Phase Diagram Calculations in Materials Processing"*, in "Control and Optimization in Minerals, Metals and Materials Processing", Edited by the Canadian Institute of Mining, Metallurgy and Petroleum, Quebec, pp.161-169, 1999.
63) M. Stan, S.Mihaiu, D.Crisan, and M.Zaharescu, *"Subsolidus Phase Equilibria in the Cu-Sb-O System", E*ur.J.Solid State Inorg.Chem., **35** (1998) 243-254.

64) M. Stan, A. Vasilescu, S. Moscu, and M. Zaharescu, *"IR Structural Characterization of the Gels in the SiO_2-P_2O_5 System"*, Rev. Roum. Chim., **43** (1998) 425-432.
65) D. P. Butt, Y. Park, M. Stan, T. C. Wallace, Sr., R. H. Hanrahan, Jr., J. C. Huling, C. L. Haertling, D. G. Kolman, and C. A. James, *"Thermal removal of Gallium from Weapons Plutonium Oxide"*, Proceedings of the Third Topical Meeting on DOE Spent Nuclear Fuel and Fissile Materials Management, September 8-11, 1998, Charleston, SC, Edited by the American Ceramic Society, Inc., pp. 556-557, 1998.
66) D. G. Kolman, C. A. James, D. P. Butt, Y. Park, and M. Stan, *"Thermally-Induced Gallium Removal From Plutonium Dioxide For MOX Fuel Production"*, Proceedings of the Third Topical Meeting on DOE Spent Nuclear Fuel and Fissile Materials Management, September 8-11, 1998, Charleston, SC, Edited by the American Ceramic Society, Inc., pp. 558-559, 1998.
67) M. Stan, S. Mihaiu, D. Crisan, and M. Zaharescu, *Subsolidus Equilibria in the Sn-Sb-Cu-O System*, Key Engineering Materials, **132/136** (1997) 790.
68) M. Stan, *"On the Three-Factor Models and the Subregular Approximation in Phase Diagram Calculation"*, CALPHAD, 19 (1995) 169–178.
69) M. Stan, *"Organizing a Relational System of Databases for Phase Diagram Calculation in Ceramic Oxide Systems"*, Proceedings of the Fourth EuroCeramics, "Basic Science", vol.2, p. 469-477, Edited by Gruppo Editoriale Faenza Editrice S. p. A., 1995.
70) A. Vasilescu, M. Stan, D. Crisan and R. Marchidan, *"Sol-gel Materials in the TiO2 – CdO System"* in "Zilele Academice Timisene", Ed. a IV-a, vol.1, pp.291-294, Ed. Mirton, Timisoara, 1995.
71) A. Vasilescu, M. Stan, R. Marchidan, and R. Popescu, *" Sol - Gel Materials in the TiO2 – Sb2O3 System "*, Proceedings of the 8th CIMTEC - World Ceramics Congress and Forum on New Materials, Florence, Italy, Edited by: P. Vicenzini, Faenza, 1995.
72) I. Teoreanu, V. Fruth, M. Zaharescu, G. Tanase, R. Popescu, M.Stan, and G. Aldica, *"The Influence of Dopants on the Formation Mechanism of the Superconducting Phases in the Bi-Sr-Ca-Cu-O System"*, Proceedings of the Third EuroCeramics, vol.2, pp 659, Ed. P. Duran, 1993.
73) M. Zaharescu, M. Raileanu, S. Mihaiu, M.Stan, and L. Constantinescu, *"Polysilicon Anions Polymerization Degree Determination"*, Rev. Chim., vol. **42** (1991) 406-410.

Seminars and Conference Presentations

1) M. Stan, *Certainty and Uncertainty at Multiple Scales, Quantification of Uncertainty in Materials Science* Workshop, Gaithersburg, MD, Jan. 14, 2016 (invited).
2) M. Stan, *Bridging Scales in Modeling and Experimentation*, The Modeling and Experimental Validation Summer School, ORNL, Aug. 20, 2016 (invited).
3) M. Stan and P. Cristea., *Certainty and Uncertainty of Thermodynamic Data*, RomPhysChem 16 Conference, Galati, Romania, Sept. 21-24, 2016 (invited).
4) M. Stan, *Materials Design for Energy Applications*, Seminar at Northwestern University, Feb. 25, 2016 (invited).
5) M. Stan, *Computational Science for Energy Applications*, Lecture at South Florida University, March 1, 2016 (invited).
6) M. Stan, Z. G. Mei, A. D. R. Andersson, J. J. Low, A. Thompson, A. Lopez Bezanilla, C. R. Stanek, C. M. Wolveron, and P. B. Littlewood, *Chemical and Heat Transport in Uranium Oxide*, CERAMICS 2015 Conference, Chicago, IL, August 17-18, 2015 (invited).
7) M. Stan, *Materials Design for Energy Applications*, ROCAM Conference, Bucharest, Romania, July 5-10, 2015 (invited).
8) L. Liang, M. Stan and M. Anitescu, *Phase Field Modeling of The Li_2O_2 Growth in a Porous Cathode in Li-Air Batteries with Organic Electrolytes*, 227th Electrochemical Society Meeting, Chicago, May 24-28, 2015.
9) M. Stan, *Nuclear Energy Advanced Modeling and Simulation (NEAMS)*, WPMM Meeting, Paris, France, May 5-7, 2015 (invited).
10) M. Stan, *Science and Cinema*, NURETH-16, Chicago, IL, Sept. 2, 2015 (invited).
11) M. Stan, *Computational Science and Cinema*, ATPESC, St. Charles, IL, Aug. 13, 2015 (invited).
12) M. Stan, *Science and Cinema*, MeV Summer School, Argonne National Laboratory, July 29, 2015 (invited).
13) M. Stan, *Modeling and Simulation Coordination at DOE Office of Nuclear Energy*, ANS Annual Meeting, Reno, NV, June 16-20, 2014 (invited).

14) 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_2*, TMS Meeting, San Diego, CA, Feb. 16-20, 2014.
15) M. Stan and Z. G. Mei, *EAM insight into the phase stability of alloys*, TMS Meeting, San Diego, CA, Feb. 16-20, 2014 (invited).
16) Z. G. Mei and M. Stan, *Computational Models of Thermodynamic Properties of Uranium Nitride*, SNA+MC 2013, Paris, France, Oct. 27-31, 2013.
17) 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.
18) Z. G. Mei and M. Stan, *Thermodynamics and Phase Stability of UN by DFT*, MMSNF 2013, Chicago, IL, Oct. 14-16, 2013.
19) M. Stan, Z. G. Mei, A. E. Thompson and C. M. Wolverton, *Thermodynamic Models of UO_2 and UN*, MMSNF 2013, Chicago, IL, Oct. 14-16, 2013 (invited).
20) 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 (invited, key note).
21) M. Stan, *Microstructural Heterogeneity and Thermal Transport*, PRICM-8 Conference, Waikoloa, HI, Aug. 4-9, 2013 (invited).
22) 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.
23) M. Stan, B. Mihaila, D. Yung, Z. G. Mei, and P. Cristea, *Heterogeneity Effects on the Thermal Conductivity of UO2+x*, TMS Meeting, San Antonio, TX, March 3-7, 2013 (invited).
24) Z. G. Mei, M. Stan, P. Cristea, and A. D. Andersson, *Defect and Diffusion in UO2±x by Quantum Mechanics and Statistical Thermodynamic Approaches*, TMS Meeting, San Antonio, TX, March 3-7, 2013.
25) M. Stan, *Controlled Heterogeneity of Reactor Materials*, NuMat 2012 Conference, Osaka, Japan, Oct 22-26, 2012 (invited, plenary).
26) M. Stan, *Multi-Scale Heat Transport and Chemical Diffusion*, MS&T Conference, Pittsburgh, PA, Oct. 8-12, 2012 (invited).
27) 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 (invited)
28) 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).
29) M. Stan, B. Mihaila, J. Crapps, and D. Yun, *Thermal and Oxygen Transport in UO2 Fuel Elements*, ANS Meeting, Chicago, IL, June 24-28, 2012.
30) M. Stan, *Multi-Scale Simulation Methods for Nuclear*, Multi-Scale Simulations of Nuclear Materials - Workshop, ANL, June 4, 2012.
31) M. Stan, *Phase Field Method Simulations of Microstructure Evolution*, Multi-Scale Simulations of Nuclear Materials - Workshop, ANL, June 4, 2012.
32) M. Stan, *Computational Microscopy*, Univ. of California Santa Barbara Seminar, Goleta, CA, April 16, 2012 (invited).
33) M. Stan, *Heterogeneity of Nuclear Fuels*, MRS Spring Meeting, San Francisco, CA, April 9-13, 2012.
34) M. Stan, *Bridging the Micro and Macro Scales*, MIT Seminar, March 20, 2012 (invited).
35) M. Stan, *Heterogeneity of Nuclear Fuels*, Materials Modeling and Simulation for Nuclear Fuels (MMSNF) workshop, Aix en Provence, France, Sept. 26-28, 2011.
36) 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.
37) M. Stan, *Materials Discovery and Design*, Seminar at the Illinois Institute of Technology, Chicago, March 28, 2011 (invited).
38) 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).
39) 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).
40) 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.

41) M. Stan, *Integration of Simulation Techniques for Nuclear Fuels*, F-BRIDGE School, JRC-ITU, Karlsruhe, Germany, Sept. 28-Oct. 2, 2010 (invited).
42) 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).
43) 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).
44) M. Stan, *Advanced Models and Simulations for Nuclear Energy,* Seminar, Argonne National Laboratory, Nov. 24, 2009 (invited).
45) M. Stan, *Models and Simulations of Materials: Results and Strategy*, Materials Science Seminar, Oak Ridge National Laboratory, Oct. 1, 2009 (invited).
46) M. Stan, *Models and Simulations of Nuclear Fuels: Results and Strateg,* Materials Models and Simulations for Nuclear Fuels (MMSNF-8) Workshop, Albuquerque, NM, Oct. 19-21, 2009.
47) 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).
48) 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).
49) 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.
50) M. Stan, *Models and Simulations for Energy Applications*, The Summer Lecture Series, Los Alamos National Laboratory, June 12, 2009 (invited).
51) 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.
52) M. Stan and B. Mihaila, *Models and Simulations of Oxide Nuclear Fuels*, THOR Energy Meeting, Portland, OR, March 27, 2009 (invited).
53) M. Stan, *Computer Simulations for Nuclear Energy Applications*, High Speed Computing Conference Salishan Lodge, Gleneden Beach, OR, April 27-30, 2009 (invited).
54) 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).
55) 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).
56) M. Stan, *Discovery and Design of Materials for Energy Applications*, Invited Seminar, Oak Ridge National Laboratory, Dec. 18, 2008 (invited).
57) M. Stan, *Discovery and Design of Advanced Nuclear Fuels*, Materials Research Society Fall Meeting, Boston MA, Dec. 1-5, 2008 (invited).
58) M. Stan, *Uncertainty Quantification Needs for Nuclear Energy Applications*, Information Science and Technology workshop, Los Alamos, Dec. 11, 2008 (invited).
59) 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).
60) M. Stan, *Modeling Phase Stability of Nuclear Fuels*, Models and Simulations for Nuclear Energy workshop, Los Alamos National Laboratory, July 29-30, 2008 (invited).
61) 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 (key-note, invited)
62) 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.
63) 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.

64) 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).
65) 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).
66) 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).
67) 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 (invited).
68) M. Stan, *Thermodynamics of Nuclear Fuel Materials*, MRS Spring Conference, San Francisco, CA, March 24-28, 2008 (invited).
69) P. Cristea and M. Stan, *Analytical Model of Defect Configurational Entropy of PuO2-x And CeO2-x*, MRS Spring Conference, San Francisco, CA, March 24-28, 2008.
70) 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).
71) M. Stan, *Models and Simulations of Advanced Nuclear Fuels and Materials*, Japan Atomic Energy Agency Seminar, Tokay, Japan, Feb. 26, 2008 (invited).
72) 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 (invited).
73) 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 (invited).
74) M. Stan, *Models and Simulations of Advanced Nuclear Fuels*, US-Japan Models and Simulations Workgroup Meeting, Tokyo, Japan, Sept. 18-19, 2007 (invited).
75) 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.
76) M. Stan, *Models and Simulations of Advanced Nuclear Fuels*, Seminar, Oak Ridge National Laboratory, Dec. 5, 2007 (invited).
77) M. Stan, *Thermodynamics of Nuclear Fuel Materials*, MRS Conference, Boston, MA, Nov. 26-30, 2007 (invited).
78) M. Stan, *Models and Simulations of Advanced Nuclear Fuels*, Advance Fuel Cycle Conference, Nizny Novogorad, Russia, Sept 24-27, 2007 (invited).
79) 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).
80) M. Stan, *The Scientific Method*, MSTea Seminar Series, Los Alamos National Laboratory, Los Alamos, NM, Aug. 28, 2007 (invited).
81) 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).
82) M. Stan, *Materials for Nuclear Energy*, Energy Council Meeting, Los Alamos National Laboratory, Los Alamos, NM, June 20, 2007 (invited).
83) 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.
84) M. Stan, *Designed Materials Overview*, Materials Capability Review, Los Alamos National Laboratory, Los Alamos, NM, May 15-18, 2007 (invited).
85) 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.
86) 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.

87) 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).
88) M. Stan, *Thermodynamics of Nuclear materials*, I-NERI Meeting, April 26-27, 2007, Aix en Provence, France (invited).
89) M. Stan, *Models of Materials Properties for Advanced Fuel Performance Codes*, CESC Meeting, Washington D. C., April 10-12, 2007 (invited).
90) M. Stan, *Current Fuel Models and Simulations Activities at LANL*, Fuel Performance Meeting Idaho National Laboratory, March. 22-23, 2007 (invited).
91) M. Stan, *Materials for Nuclear Energy Applications*, TMS Conference, Orlando, FL, Feb. 26-March 1, 2007 (invited).
92) 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.
93) M. Stan, *Advanced Fuel Performance Codes*, CEA meeting, Cadarache, France, Dec. 6, 2006 (invited).
94) M. Stan, *Models and Simulations of Thermodynamic Properties and Transport Phenomena in UO2+x*, International Information Exchange Meeting on Thermodynamics of Nuclear Fuels, Saclay, Franc, Nov. 27-Dec. 1, 2006 (invited).
95) 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.
96) 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.
97) M. Stan, *Nuclear Fuel Performance Codes Status and Requirements*, Workshop on Nuclear Fuel Performance, Washington DC, Nov. 8, 2006 (invited).
98) M. Stan, *Thermodynamics of Roses-Toward Predictive Models and Simulations*, Materials Research Seminar, Louisiana State University, Baton Rouge, LA, Oct. 27, 2006 (invited).
99) 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).
100) M. Stan, *Thermodynamics of Nuclear Materials*, Romanian Conference on Advanced Materials, ROCAM 2006, Bucharest, Romania, Sept. 9-10, 2006 (invited).
101) 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).
102) 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).
103) 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).
104) 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)
105) 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).
106) 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.
107) 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.
108) 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).
109) 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).
110) M. Stan, *Models and Simulations of Thermodynamic Properties of Nuclear Fuels*, LANL-CEA meeting, Saclay, France, June 5-9, 2006 (invited).

111) J. C. Ramirez, P. Cristea, and M. Stan, *Simulations Of Heat and Oxygen Diffusion in UO2 Nuclear Fuel Rods*, MMSNF 5 workshop, Nice, France, June 1-2, 2006.
112) 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).
113) 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.
114) M. Stan, *Thermodynamics of Roses*, TMS 2006 135th Annual Meeting & Exhibition, San Antonio, TX, March 12-16, 2006 (invited).
115) M.I. Baskes, S.Y. Hu and M. Stan, *Calculated Properties of Pu-Ga Alloys Using the Modified Embedded Atom Method*, TMS 2006 135th Annual Meeting & Exhibition, San Antonio, TX, March 12-16, 2006 (invited).
116) 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 135th Annual Meeting & Exhibition, San Antonio, TX, March 12-16, 2006.
117) 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)
118) 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.
119) 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.
120) 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.
121) M. Stan, *The Entropy of Delta Pu-Ga Alloys*, ANS Annual Meeting San Diego, CA, June 5-9, 2005.
122) 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).
123) M. Stan, *The Entropy of Alloys*, 2005 TMS Annual Meeting & Exhibition, San Francisco, CA, Feb. 13-17, 2005.
124) P. Cristea and M. Stan, *Oxygen Diffusivity in Nonstoichiometric Cerium Dioxide*, 2005 TMS Annual Meeting & Exhibition, San Francisco, CA, Feb. 13-17, 2005.
125) M. Stan, *Prediction of Nuclear Fuel Materials Properties*, American Nuclear Society Winter Meeting, Washington DC, Nov. 14-18, 2004.
126) M. Stan and P. Cristea, *Thermochemistry of Defects and Oxygen Diffusion in PuO2-x*, American Nuclear Society Winter Meeting, Washington DC, Nov. 14-18, 2004.
127) 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.
128) P. Cristea, M. Stan, T. C. Wallace, Sr., and K. V. Woan, *Controlling Nonstoichiometry of PuO2-x and UO2+x*, Materials Models and Simulations for Nuclear Fuels Workshop (MMSNF-3), Washington DC, Nov. 18-19, 2004.
129) 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.
130) M. Stan, *The Entropy of Alloys*, TOFA 2004-Discussion Meeting on Thermodynamics of Alloys, Vienna, Austria, Sept. 12 - 17, 2004.
131) M. Stan, P. Cristea, T. C. Wallace, Sr., *Defect Thermochemistry and Phase Stability in PuO2-x*, 11th Symposium on Thermodynamics of Nuclear Materials (STNM11), Karlsruhe, Germany, Sept. 6-10, 2004.
132) 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.
133) M. Stan, *Thermochemistry of Defects and Oxygen Diffusion in PuO2-x*, U.S. – Russian Plutonium Science Workshop, Sarov, Russia, Aug. 30-Sept. 2, 2004.
134) 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).
135) M. Stan, S. Swaminarayan, and K. Lam, *Chemical Reaction Models in Truchas*, TRUCHAS Workshop, Los Alamos, NM, June 21-24, 2004.

136) 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.

137) 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.

138) 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.

139) 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.

140) 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).

141) 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.

142) 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.

143) 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.

144) 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.

145) 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.

146) Conference: 4th Pacific Rim International Conference on Advanced Materials and Processing (PRICM4); Honolulu, HI, Dec. 11-15, 2001.

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