Mark Asta

Department of Materials Science and Engineering
University of California, Berkeley
Email: mdasta@berkeley.edu
URL: http://asta.mse.berkeley.edu/

EDUCATION

Ph.D. in interdisciplinary program combining Physics and Materials Science and Engineering, University of California at Berkeley, October 1993

Master of Arts in Physics, University of California at Berkeley, December 1990

Bachelor of Science in Engineering Physics, University of California at Berkeley, May 1988

PROFESSIONAL EXPERIENCE

University of California, Berkeley, CA
- College of Engineering:
  - January, 2023 – present: Executive Associate Dean
  - February, 2023 – present: Shankar Sastry Chair for Leadership and Innovation
- Department of Materials Science and Engineering:
  - January, 2010 – present: Professor
  - July, 2012 – January, 2018: Department Chair
  - July, 2015 – present: Arthur C. and Phyllis G. Oppenheimer Professor in Advanced Materials Analysis

Lawrence Berkeley National Laboratory, Berkeley, CA
- Materials Sciences Division:
  - April, 2010 – February, 2023: Faculty Scientist
  - January, 2018 – December, 2022: Division Director
  - February, 2023 – Present: Faculty Senior Scientist

University of California, Davis, CA
- Department of Chemical Engineering and Materials Science:
  - October, 2005 – October, 2009: Professor
  - July, 2008 – October, 2009: Vice Chair
  - October, 2009 – June, 2016: Adjunct Professor

Northwestern University, Evanston, IL
- Department of Materials Science and Engineering:
  - January, 2000 – September, 2005: Associate Professor

Sandia National Laboratories, Livermore, CA:
- October, 1993 - February, 1995: Postdoctoral Associate
- February, 1995 – December, 1999: Senior Member of the Technical Staff

AWARDS AND HONORS

1. ASM International's Materials Science Research Silver Medal, 2002.
2. Department of Materials Science and Engineering "Teacher of the Year," Northwestern University, 2004.
3. Fellow of the American Physical Society, 2010.
4. TMS (The Minerals, Metals & Materials Society) Electronic, Magnetic, and Photonic Materials Division (EMPMD) Distinguished Scientist/Engineer Award, 2013.
5. TMS William Hume-Rothery Award, 2019.
6. TMS Fellow, 2020.
7. ASM International J. Willard Gibbs Phase Equilibria Award, 2020.
8. David Turnbull Lectureship Award, Materials Research Society, 2023.

PATENTS

"A method for Enhancing the solubility of B and In in Si," B. Sadigh, T. Lenosky, T. Diaz de la Rubia, M. Giles, M.-J. Caturla, V. Ozolins, **M. Asta**, V. Ozolins, S. Theiss, M. Foad, and Andrew Quong, U. S. Patent 6,498,078 B2, December 24, 2002.

PUBLICATIONS

(34217 Citations, h-index=92, based on *Google Scholar,* December 31, 2023)

Refereed Journals

1. G. Ceder, **M. Asta**, W.C. Carter, M. Kraitchman, D. de Fontaine, M.E. Mann, and M. Sluiter, "Phase Diagram and Low-Temperature Behavior of Oxygen Ordering in $YBa_2Cu_3O_z$ Using *ab Initio* Interactions," Physical Review B Vol. 41, 8698 (1990).
2. D. de Fontaine, G. Ceder, and **M. Asta**, "Low-Temperature Long-Range Oxygen Order in $YBa_2Cu_3O_z$," Nature Vol. 343, 544 (1990).
3. D. de Fontaine, G. Ceder, and **M. Asta**, "Thermodynamics of Oxygen Ordering in $YBa_2Cu_3O_z$," Journal of Less-Common Metals Vol. 164&165, 108 (1990).
4. **M. Asta**, D. de Fontaine, G. Ceder, E. Salomons, and M. Kraitchman, "One- and Two-Dimensional Oxygen Ordering in $YBa_2Cu_3O_z$," Journal of Less-Common Metals Vol. 168, 39 (1991).
5. **M. Asta**, G. Ceder, and D. de Fontaine, "Comment on 'Nucleated and Continuous Ordering in CuAu'," Physical Review Letters Vol. 66, 1798 (1991).
6. **M. Asta**, C. Wolverton, D. de Fontaine, and H. Dreyssé, "Effective Cluster Interactions from Cluster Variation Formalism - I," Physical Review B Vol. 44, 4907 (1991).
7. G. Ceder, **M. Asta**, and D. de Fontaine, "Computation of the OI-OII-OIII Phase Diagram and Local Oxygen Configurations for $YBa_2Cu_3O_z$ with z between 6.5 and 7," Physica C Vol. 177, 106 (1991).

8. C. Wolverton, **M. Asta**, H. Dreyssé, and D. de Fontaine, "Effective Cluster Interactions from Cluster Variation Formalism - II," Physical Review B Vol. 44, 4914 (1991).

9. **M. Asta**, D. de Fontaine, M. van Schilfgaarde, M. Sluiter, and M. Methfessel, "First-Principles Phase Stability Study of fcc Alloys in the Ti-Al System," Physical Review B Vol. 46, 5055 (1992).

10. D. de Fontaine, C. Wolverton, **M. Asta**, and G. Ceder, "Prediction of Ordered Superstructure Phase Equilibria," Journal of Phase Equilibria Vol. 13, 344 (1992).

11. D. de Fontaine, **M. Asta**, G. Ceder, R. McCormack, and G. Van Tendeloo, "On the Asymmetric Next-Nearest-Neighbor Ising Model of Oxygen Ordering in $YBa_2Cu_3O_z$," Europhysics Letters Vol. 19, 229 (1992).

12. **M. Asta**, R. McCormack, and D. de Fontaine, "Theoretical Study of Alloy Phase Stability in the Cd-Mg System," Physical Review B Vol. 48, 748 (1993).

13. **M. Asta**, D. de Fontaine, and M. van Schilfgaarde, "First-Principles Study of Phase Stability of Ti-Al Intermetallic Compounds," Journal of Materials Research Vol. 8, 2554 (1993).

14. C. Wolverton, **M. Asta**, S. Ouannasser, H. Dreyssé, and D. de Fontaine, "New Developments in the *ab Initio* Determination of Transition Metal Alloy Phase Diagrams," J. Chim. Phys. Vol. 90, 249 (1993).

15. R. McCormack, **M. Asta**, D. de Fontaine, G. Garbulsky, and G. Ceder, "The hcp Ising Model in the Cluster Variation Approximation," Physical Review B Vol. 48, 6767-6780 (1993).

16. **M. Asta** and S. M. Foiles, "Embedded-Atom-Method, Effective-Pair-Interaction Study of the Structural and Thermodynamic Properties of Cu-Ni, Cu-Ag and Au-Ni Solid Solutions," Physical Review B Vol. 53, 2389-2404 (1996).

17. **M. Asta**, "Theoretical Study of the Thermodynamic Properties of α-δ' Interphase Boundaries in Al-Li," Acta Materialia Vol. 44, 4131 (1996).

18. **M. Asta** and D. D. Johnson, "Thermodynamic Properties of FCC-Based Al-Ag Alloys," Computational Materials Science Vol. 8, 64 (1997).

19. **M. Asta** and A. A. Quong, "The Concentration and Temperature Dependences of Antiphase-Boundary Energies in γ-TiAl: a First-Principles Study," Philosophical Magazine Letters Vol. 76, 331 (1997).

20. R. McCormack, **M. Asta**, J. J. Hoyt, B. C. Chakoumakos, S. T. Misture, J. D. Althoff and D. D. Johnson, "Experimental and Theoretical Investigations of Order-Disorder in Cu_2AlMn," Computational Materials Science Vol. 8, 39 (1997).

21. D. D. Johnson and **M. Asta**, "Energetics of Homogeneously-Random FCC Al-Ag Alloys: A Detailed Comparison of Computational Methods," Computational Materials Science Vol. 8, 54 (1997).

22. D. Morgan, D. de Fontaine and **M. Asta**, "Towards a Total Energy Tight-Binding Hamiltonian Based upon the Linear-Muffin-Tin-Orbital Method," Computational Materials Science Vol. 8, 122 (1997).

23. J. D. Althoff, D. Morgan, D. de Fontaine, **M. Asta**, S. M. Foiles and D. D. Johnson, "Vibrational Spectra in Ordered and Disordered Ni_3Al," Physical Review B, Rapid Communication, Vol. 56, R5705 (1997).

24. **M. Asta**, S. M. Foiles and A. A. Quong, "First-Principles Calculations of Bulk and Interfacial Thermodynamic Properties for FCC-Based Al-Sc Alloys," Physical Review B Vol. 57, 11265-11275 (1998).

25. J. D. Althoff, D. Morgan, D. de Fontaine, **M. Asta**, S. M. Foiles and D. D. Johnson, "Embedded-Atom Method Calculations of Vibrational Thermodyamic Properties of Ordered and Disordered Ni_3Al," Computational Materials Science Vol. 10, 411 (1998).

26. R. W. Hyland, Jr., **M. Asta**, C. L. Rohrer, and S. M. Foiles, "Al(fcc):$Al_3Sc(L1_2)$ Interphase Boundary Energy Calculations," Acta Materialia Vol. 46, 3667 (1998).

27. P. D. Tepesch, **M. Asta** and G. Ceder, "Computation of Configurational Entropy Using Monte Carlo Probabilities in Cluster-Variation-Method Entropy Expressions," Modelling and Simulation in Materials Science and Engineering Vol. 6, 787 (1998).

28. **M. Asta**, D. Morgan, J. J. Hoyt, B. Sadigh, J. D. Althoff, D. de Fontaine and S. M. Foiles, "Embedded-Atom-Method Study of Structural, Thermodynamic, and Atom-Transport Properties of Liquid Ni-Al Alloys," Physical Review B Vol. 59, 14271 (1999).

29. D. D. Johnson, **M. Asta** and J. D. Althoff, "Temperature-Dependent Chemical Ordering in BCC-Based Ternary Alloys: a Theoretical Study in Ti-Al-Nb," Philosophical Magazine Letters Vol. 79, 551 (1999).

30. B. Sadigh, **M. Asta**, V. Ozolins, A. K. Schmid, N. C. Bartelt, A. A. Quong and R. Q. Hwang, "Short-Range Order and Phase Stability of Surface Alloys: PdAu on Ru(0001)," Physical Review Letters Vol. 83, 1379 (1999).

31. J. J. Hoyt, B. Sadigh, **M. Asta** and S. M. Foiles, "Kinetic Phase Field Parameters for the Cu-Ni System Derived from Atomistic Computations," Acta Materialia, Vol. 47, 3181 (1999).

32. **M. Asta** and J. J. Hoyt, "Thermodynamic Properties of Coherent Interfaces in FCC-Based Ag-Al Alloys: A First-Principles Study," Acta Materialia, Vol. 48, 1089-1096 (2000).

33. J. J. Hoyt, **M. Asta**, and B. Sadigh, "A Test of the Universal Scaling Law for the Diffusion Coefficient in Liquids," Physical Review Letters, Vol. 85, 594-597 (2000).

34. **M. Asta**, V. Ozolins and J. J. Hoyt, "The Energetics of Surface-Alloy Formation: an Embedded-Atom-Method, Second-Order-Expansion Study," Modelling and Simulation in Materials Science and Engineering, Vol. 8, 287-293 (2000).

35. V. Ozolins and **M. Asta**, "Large Vibrational Effects on Calculated Phase Boundaries in Al-Sc," Physical Review Letters, Vol. 86, 448 (2001).

36. G. E. Thayer, V. Ozolins, A. K. Schmid, N. C. Bartelt, **M. Asta**, J. J. Hoyt, S. Chiang, and R. Q. Hwang, "Role of Stress in Thin Film Alloy Thermodynamics: Competition Between Alloying and Dislocation Formation," Physical Review Letters, Vol. 86, 660-663 (2001).

37. C. Woodward, **M. Asta**, G. Kresse, and J. Hafner, "Density of Constitutional and Thermal Point Defects in $L1_2$ Al_3Sc," Physical Review B, Vol. 63, 094103:1-6 (2001).

38. M. I. Baskes, **M. Asta**, and S. G. Srinivasan, "Using First-Principles Calculations to Determine the Range of Forces in Empirical Many-Body Potentials," Philosophical Magazine A, Vol. 81, 991-1008 (2001).

39. J. J. Hoyt, **M. Asta** and A. Karma, "A Method for Calculating the Anisotropy of the Solid-Liquid Interfacial Free Energy," Physical Review Letters, Vol. 86, 5530-5533 (2001).

40. **M. Asta**, V. Ozolins, J. J. Hoyt, M. van Schilfgaarde, "Ab Initio Molecular Dynamics Study of Highly Non-Ideal Structural and Thermodynamic Properties of Liquid Ni-Al Alloys," Physical Review B: Rapid Communications, Vol. 64, 020201:1-4 (2001).

41. **M. Asta** and V. Ozolins, "Structural, Vibrational, and Thermodynamic Properties of Al-Sc Alloys and Intermetallic Compounds," Physical Review B Vol. 64, 094104:1-14 (2001).

42. A. Van der Ven, G. Ceder, **M. Asta** and P. D. Tepesch, "First-Principles Theory of Ionic Diffusion with Nondilute Carriers," Physical Review B, Vol. 64, 184307:1-17 (2001).

43. A. van de Walle and **M. Asta**, "First-Principles Investigation of Perfect and Diffuse Antiphase Boundaries in HCP-Based Ti-Al Alloys," Metallurgical Transactions, Vol. 33A, 735 (2002).

44. V. Ozolins, **M. Asta** and J. J. Hoyt, "Elastic Relaxations in Ultrathin Alloy Films," Physical Review Letters, Vol. 88, 096101 (2002).

45. B. Krack, V. Ozolins, **M. Asta**, and I. Daruka, "`Devil's Staircases' in Bulk-Immiscible Ultrathin Alloy Films," Physical Review Letters, Vol. 88, 186101 (2002).

46. H. Ramalingam, **M. Asta**, A. van de Walle, and J. J. Hoyt, "Atomic-Scale Simulation Study of Equilibrium Solute Adsorption at Alloy Solid-Liquid Interfaces," Interface Science, Vol. 10, 149 (2002).

47. J. J. Hoyt, **M. Asta** and A. Karma, "Atomistic Simulation Methods for Computing the Kinetic Coefficient in Solid-Liquid Systems," Interface Science, Vol. 10, 181 (2002).

48. J. J. Hoyt and **M. Asta**, "An Atomistic Computation of the Liquid Diffusivity, the Solid-Liquid Interfacial Free Energy and the Kinetic Coefficient in Au and Ag," Physical Review B, Vol. 65, 214106:1-11 (2002).

49. A. van de Walle and **M. Asta**, "Self-Driven Lattice-Monte-Carlo Simulations of Alloy Thermodynamic Properties and Phase Diagrams," Modelling and Simulation in Materials Science and Engineering, Vol. 10, 521-538 (2002).

50. N. Erdman, K. R. Poeppelmeier, **M. Asta**, O. Warschkow, D. E. Ellis and L. D. Marks, "The Structure and Chemistry of the TiO_2-rich Surface of $SrTiO_3$ (001)," Nature, Vol. 419, 55-58 (2002).

51. **M. Asta**, J. J. Hoyt and A. Karma, "Calculation of Alloy Solid-Liquid Interfacial Free Energies from Atomic-Scale Simulations," Physical Review B, Vol. 66, 100101:1-4 (2002).

52. A. van de Walle, **M. Asta** and G. Ceder, "The Alloy Theoretic Automated Toolkit: A User Guide," CALPHAD, Vol. 26, 539-553 (2002).

53. G. Ghosh, A. van de Walle, **M. Asta** and G. B. Olson, "Phase Stability of the Hf-Nb System: From First-Principles to CALPHAD," CALPHAD, Vol. 26, 491-511 (2002).

54. A. van de Walle, **M. Asta** and P. W. Voorhees, "First-principles calculation of the effect of strain on the diffusion of Ge adatoms on Si and Ge (001) surfaces," Physical Review B, Vol. 67, 041308 (2003).

55. J. J. Hoyt, J. W. Garvin, E. B. Webb and **M. Asta**, "An Atomistic Embedded Atom Method Interatomic Potential for the Cu-Pb System," Modelling and Simulation in Materials Science and Engineering, Vol. 11, 287-299 (2003).

56. E. A. Marquis, D. N. Seidman, **M. Asta**, C. Woodward and V. Ozolins, "Equilibrium Mg Segregation at Al/Al_3Sc Heterophase Interfaces on an Atomic Scale: Experiments and Computations," Physical Review Letters, Vol. 91, 036101 (2003).

57. N. Erdman, O. Warschkow, **M. Asta**, K. R. Poeppelmeier, D. E. Ellis and L. D. Marks, "Surface Structures of $SrTiO_3$(001): A $Ti0_2$-rich Reconstruction with a c(4x2) Unit Cell," J. Am. Chem. Soc., Vol. 125, 10050-10056 (2003).

58. J. J. Hoyt, **M. Asta** and A. Karma, "Atomistic and Continuum Modeling of Dendrite Solidification," Materials Science and Engineering R, Vol. 41, 121-163 (2003).

59. M. I. Mendelev, S. Han, D. J. Srolovitz, G. J. Ackland, D. Y. Sun and **M. Asta**, "Development of New Interatomic Potentials Appropriate for Crystalline and Liquid Iron," Philosophical Magazine, Vol. 83, pp. 3977-3994 (2003).

60. D. Y. Sun, **M. Asta**, J. J. Hoyt, M. I. Mendelev and D. J. Srolovitz, "Crystal-Melt Interfacial Free Energies in Metals: FCC vs. BCC," Physical Review B, Vol. 69, 020102(R) (2004).

61. D. Y. Sun, **M. Asta**, and J. J. Hoyt, "Kinetic Coefficient of Ni Solid-Liquid Interfaces from Molecular Dynamics Simulations," Physical Review B, Vol. 69, 024108 (2004).

62. C. Wolverton, V. Ozolins and **M. Asta**, "Hydrogen in Aluminum: First-Principles Calculations of Structure and Thermodynamics," Physical Review B, Vol. 69, 144109 (2004).

63. D. Y. Sun, **M. Asta**, and J. J. Hoyt, "Crystal-Melt Interfacial Free Energies and Mobilities in FCC and BCC Fe," Physical Review B, Vol. 69, 174103 (2004).

64. M. J. Beck, A. van de Walle and **M. Asta**, "Ge on Si(100) Wetting Layer Surface Energetics and Structure," Physical Review B, Vol. 70, 205337 (2004).

65. O. Warschkow, **M. Asta**, N. Erdman, K.R. Poeppelmeier, D.E. Ellis and L.D. Marks, "TiO_2-rich Reconstructions of $SrTiO_3$(001): A Theoretical Study of Structural Patterns," Surface Science, Vol. 573, 446-456 (2004).

66. K. Thornton and **M. Asta**, "Current Status and Outlook of Computational Materials Science Education in the U. S.," Modeling and Simulation in Materials Science and Engineering, Vol. 13, R1-R17 (2005).

67. R. Benedek, A. van de Walle, S. S. A. Gerstl, **M. Asta**, D. N. Seidman, and C. Woodward, "Partitioning of Impurities in Multi-Phase TiAl Alloys," Physical Review B, Vol. 71, 094201 (2005).

68. V. Ozolins, B. Sadigh and **M. Asta**, "Effects of Vibrational Entropy on the Al-Si Phase Diagram," Journal of Physics – Condensed Matter, Vol. 17, 1-14 (2005).

69. O. E. Shklyaev, M. J. Beck, **M. Asta**, M. J. Miksis and P. W. Voorhees, "Role of Strain-Dependent Surface Energies in Ge/Si(001) Island Formation," Physical Review Letters, Vol. 94, 176102 (2005).

70. G. Ghosh and **M. Asta**, "First-Principles Calculation of Structural Energetics of Al-TM (TM=Ti, Zr, Hf) Intermetallics," Acta Materialia, Vol. 53, 3225-3252 (2005).

71. Bo Yang, **M. Asta**, O. N. Mryasov, T. Klemmer and R. W. Chantrell, "Monte-Carlo-Simulation Study of A1-$L1_0$ Ordering Transitions in FePt Nanoparticles," Scripta Materialia, Vol. 53, 417-422 (2005).

72. J. Z. Liu, A. van de Walle, G. Ghosh and **M. Asta**, "Structure, Energetics and Mechanical Stability of Fe-Cu bcc Alloys from First-Principles Calculations," Physical Review B, Vol. 72, 144109 (2005).

73. G. Ghosh and **M. Asta**, "Phase Stability, Phase Transformations, and Elastic Properties of Cu_6Sn_5: Ab Initio Calculations and Experimental Results," Journal of Materials Research, Vol. 20, 3102-3117 (2005).

74. H. Reichert, A. Schöps, I. B. Ramsteiner, V. N. Bugaev, O. Shchyglo, A. Udyansky, H. Dosch, **M. Asta**, R. Drautz and V. Honkimäki, "Competition Between Order and Phase Separation in Au-Ni," Physical Review Letters, Vol. 95, 235703 (2005).

75. E. A. Marquis, **M. Asta**, D. N. Seidman and C. Woodward, "Composition Evolution of Nanoscale Al_3Sc Precipitates in an Al-Mg-Sc Alloy," Acta Materialia, Vol. 54, 119-130 (2006).

76. W. Cao, J. Zhu, F. Zhang, W. A. Oates, **M. Asta** and Y. A. Chang, "Application of the Cluster/Site Approximation to the Calculation of Coherent Interphase Boundary Energetics," Acta Materialia, Vol. 54, 377-383 (2006).

77. D. Y. Sun, M. I. Mendelev, C. A. Becker, K. Kudin, Tomorr Haxhimali, **M. Asta**, J. J. Hoyt, A. Karma and D. J. Srolovitz, "Crystal-Melt Interfacial Free Energies in HCP Metals: A Molecular Dynamics Study of Mg," Phys. Rev. B, Vol. 73, 024116 (2006).

78. Kuo-An Wu, A. Karma, J. J. Hoyt and **M. Asta**, "Ginzburg-Landau Theory of Crystalline Anisotropy for BCC-Liquid Interfaces," Phys. Rev. B, Vol. 73, 094101 (2006).

79. C. J. Moore, C. M. Retford, M. J. Beck, **M. Asta**, M. J. Miksis, and P. W. Voorhees, "Orientation Dependence of Strained-Ge Surface Energies Near (001): Role of Dimer-Vacancy-Lines and Their Interactions with Steps," Phys. Rev. Lett., Vol. 96, 126101 (2006).

80. C. A. Becker, **M. Asta**, J. J. Hoyt and S. M. Foiles, "Equilibrium Adsorption at Crystal-Melt Interfaces in Lennard-Jones Alloys from Monte-Carlo Simulations," J. Chem. Phys., Vol. 124, 164708 (2006).

81. J. J. Hoyt, **M. Asta** and D. Y. Sun, "Molecular Dynamics Simulations of the Crystal-Melt Interfacial Free Energy and Mobility in Mo and V," Philosophical Magazine, Vol. 86, 3651-3664 (2006).

82. B. Yang, **M. Asta**, O. N. Mryasov, T. J. Klemmer and R. W. Chantrell, "The Nature of A1-$L1_0$ Ordering Transitions in Alloy Nanoparticles: A Monte-Carlo Study," Acta Mater. 54, 4201-4211 (2006).

83. G. Ghosh, S. Delsante, G. Borzone, **M. Asta** and R. Ferro, "Phase Stability and Cohesive Properties of Ti-Zn Intermetallics: First-Principles Calculations and Experimental Results," Acta Mater. 54, 4977-4997 (2006).

84. G. Ghosh, S. Vaynman, **M. Asta** and M. E. Fine, "Stability and Elastic Properties of $L1_2$-$(Al,Cu)_3(Ti,Zr)$ Phases: Ab Initio Calculations and Experiments," Intermetallics 15, 44-54 (2007).

85. Z. G. Xia, D. Y. Sun, **M. Asta** and J. J. Hoyt, "Molecular Dynamics Calculations of the Crystal-Melt Interfacial Mobility for Hexagonal-Close-Packed Mg," Phys. Rev. B 75, 012103 (2007).

86. C. M. Retford, **M. Asta**, M. J. Miksis, P. W. Voorhees and E. B. Webb III, "Reconstruction and Formation Energy of Ge (105) Quantum Wires on Si (001)," Phys. Rev. B 75, 075311 (2007).

87. C. A. Becker, D. Olmsted, **M. Asta**, J. J. Hoyt, and S. M. Foiles, "Atomistic Underpinnings for Orientation Selection in Alloy Dendritic Growth," Phys. Rev. Lett. 98, 125701 (2007).

88. J. Z. Liu, G. Ghosh, A. van de Walle and **M. Asta**, "Transferable Force-Constant Modeling of Vibrational Thermodynamic Properties in FCC-Based Al-TM (TM=Ti, Zr, Hf) Alloys," Phys. Rev. B 75, 104117 (2007).

89. G. Ghosh, A. van de Walle and **M. Asta**, "First-Principles Phase Stability Calculations of Pseudobinary Alloys of $(Al,Zn)_3Ti$ with $L1_2$, $D0_{22}$ and $D0_{23}$ Structures," J. Phase Equilibria and Diffusion 28, 9-22 (2007).

90. C. A. Becker, D. Buta, J. J. Hoyt and **M. Asta**, "Crystal-Melt Interface Stresses: Atomistic Simulation Calculations for a Lennard-Jones Alloy, Stillinger-Weber Si, and Embedded Atom Method Ni," Phys. Rev. E 75, 061610 (2007).

91. D. Buta, **M. Asta** and J. J. Hoyt, "Kinetic Coefficient of Steps at the Si(111) Crystal-Melt Interface from Molecular Dynamics Simulations," J. Chem. Phys. 127, 074703 (2007).

92. M. E. Fine, J. Z. Liu and **M. D. Asta**, "An Unsolved Mystery: The Composition of BCC Cu Alloy Precipitates in BCC Fe and Steels," Mat. Sci. Engin. A 463, 271-274 (2007).

93. C. H. Lanier, A. van de Walle, N. Erdman, E. Landree, O. Warschkow, A. Kazimirov, K. R. Poeppelmeier, J. Zegenhagen, **M. Asta** and L. D. Marks, "The c(6x2) Reconstruction of the $SrTiO_3$ (001) Surface," Phys. Rev. B 76, 045421 (2007).

94. M. E. Manley, **M. Asta**, J. C. Lashley, C. M. Retford, W. L. Hults, R. D. Taylor, D. J. Thoma, J. L. Smith, R. E. Hackenberg and K. Littrell, "Soft-Phonon Feature, Site Defects, and a Frustrated Phase Transition in $Ni_{50}Ti_{47}Fe_3$: Experiments and First-Principles Calculations," Phys. Rev. B 77, 024201 (2008).

95. O. Warschkow, Y. Wang, A. Subramanian, **M. Asta** and L. D. Marks, "Structure and Local-Equilibrium Thermodynamics of the c(2x2) Reconstruction of Rutile TiO_2 (100)," Phys. Rev. Lett. 100, 086192 (2008).

96. B. Yang, T. Muppidi, V. Ozolins and **M. Asta**, "First-Principles Theory of Nanoscale Pattern Formation in Ultrathin Alloy Films: A Comparative Study of Fe-Ag on Ru(0001) and Mo(110) Substrates," Phys. Rev. B 77, 205408 (2008).

97. G. Ghosh, A. van de Walle, and **M. Asta**, "First-Principles Calculations of Structural and Energetic Properties of BCC, FCC and HCP Solid Solutions in the Al-TM (TM=Ti,Zr,Hf) Systems: A Comparison of Cluster Expansion and Supercell Methods," Acta Mater. 56, 3202-3221 (2008).

98. M. I. Mendelev, M. J. Kramer, C. A. Becker and **M. Asta**, "Analysis of Semi-Empirical Interatomic Potentials Appropriate for Simulation of Crystalline and Liquid Al and Cu," Phil. Mag. 88, 1723-1750 (2008).

99. B. Yang, T. Muppidi, V. Ozolins and **M. Asta**, "Strong Effect of Substrate Symmetry and Pre-Patterning on Self-Assembly of Compositional Patterns," Surf. Sci. 602, L123-L126 (2008).

100. D. Buta, **M. Asta** and J. J. Hoyt, "Structure and Dynamics of a Faceted Crystal-Melt Interface," Phys. Rev. E 78, 031605 (2008).

101. S. Angioletti-Uberti, **M. Asta**, M. W. Finnis and P. D. Lee, "Solid-Liquid Phase Equilibria from Free Energy Perturbation Calculations," Phys. Rev. B 78, 134203 (2008).

102. **M. Asta**, C. Beckermann, A. Karma, W. Kurz, R. Napolitano, M. Plapp, G. Purdy, M. Rappaz, and R. Trivedi, "Solidification Microstructures and Solid State Parallels: Recent Developments, Future Directions," Acta Mater. 57, 941-971 (2009).

103. J. J. Hoyt, D. Olmsted, S. Jindal, **M. Asta**, and A. Karma, "Method for Computing Short-Range Forces Driving Grain Boundary Premelting," Phys. Rev. E 79, 020601(R) (2009).

104. C. A. Becker, D. L. Olmsted, **M. Asta**, J. J. Hoyt and S. M. Foiles, "Atomistic Simulations of Crystal-Melt Interfaces in a Model Binary Alloy: Interfacial Free Energies, Adsorption Coefficients and Excess Entropy," Phys. Rev. B 79, 054109 (2009).

105. M. D. Rossell, R. Erni, **M. Asta**, V. Radmilovic and U. Dahmen, "Atomic-Resolution Imaging of Lithium in Al_3Li Precipitates," Phys. Rev. B 80, 024110 (2009).

106. B. B. Laird, R. L. Davidchack, Y. Yang and **M. Asta**, "Determination of the Solid-Liquid Interfacial Free Energy Along a Coexistence Line by Gibbs-Cahn Integration," J. Chem. Phys. 131, 114110 (2009).

107. T. Haxhimali, D. Buta, **M. Asta**, P. W. Voorhees and J. J. Hoyt, "Size-Dependent Nucleation Kinetics at Non-planar Nanowire Growth Interfaces," Phys. Rev. E 80, 050601(R) (2009).

108. M. I. Mendelev, **M. Asta**, M. J. Rahman and J. J. Hoyt, "Development of Interatomic Potentials Appropriate for Simulation of Solid-Liquid Interface Properties in Al-Mg Alloys," Phil. Mag. 89, 3269-3285 (2009).

109. J. Monk, Y. Yang, M. I. Mendelev, **M. Asta**, J. J. Hoyt, and D. Y. Sun, "Determination of the Crystal-Melt Interface Kinetic Coefficient from Molecular-Dynamics Simulations," Modelling Simul. Mater. Sci. Eng. 18, 015004 (2010). *Selected as one of ten manuscripts included in list of MSMSE "Highlights of 2010*."

110. Y. Mishin, **M. Asta** and J. Li, "Atomistic Modeling of Interfaces and Their Impact on Microstructure and Properties," Acta Mater. 58, 1117-1151 (2010).

111. S. Huang, D. L. Worthington, **M. Asta**, V. Ozolins, G. Ghosh and P. K. Liaw, "Calculation of Impurity Diffusivities in α-Fe Using First-Principles Methods," Acta Mater. 58, 1982-1993 (2010).

112. S. J. Fensin, D. Olmsted, D. Buta, **M. Asta**, A. Karma and J. J. Hoyt, "Structural Disjoining Potential for Grain Boundary Premelting and Grain Coalescence from Molecular-Dynamics Simulations," Phys. Rev. E 81, 031601 (2010).

113. H. Song, S. J. Fensin, **M. Asta**, and J. J. Hoyt, "A Molecular Dynamics Simulation of (110) Surface Premelting in Ni," Scripta Mater. 63, 128-131 (2010).

114. C. Woodward, **M. Asta**, D. R. Trinkle, J. Lill and S. Angioletti-Uberti, "Ab-Initio Simulations of Molten Ni Alloys," J. Appl. Phys. 107, 113522 (2010).

115. Y. Yang, Y. F. Gao, D. Y. Sun, **M. Asta** and J. J. Hoyt, "Capillary force-induced structural deformation in liquid infiltrated elastic circular tubes," Phys. Rev. B 81, 241407(R) (2010).

116. B. Jeon, **M. Asta**, S. M. Valone, N. Gronbech-Jensen, "Simulation of Ion-Track Ranges in Uranium Oxide," Nucl. Instr. and Meth. B 268, 2688-2693 (2010).

117. W. Morris, B. Leung, H. Furukawa, O. K. Yaghi, N. He, H. Hayashi, Y. Houndonougbo, **M. Asta**, B. B. Laird and O. M. Yaghi, "A Combined Experimental-Computational Investigation of Carbon Dioxide Capture in a Series of Isoreticular Zeolitic Imidazolate Frameworks," J. Am. Chem. Soc. 132, 11006-11008 (2010).

118. M. I. Mendelev, M. J. Rahman, J. J. Hoyt and **M. Asta**, "Molecular Dynamics Study of Solid-Liquid Interface Migration in fcc Metals," Modelling Simul. Mater. Sci. Eng. 18, 074002 (2010).

119. Y. F. Gao, Y. Yang, D. Y. Sun, **M. Asta** and J. J. Hoyt, "Molecular Dynamics Simulations of the Crystal-Melt Interface Mobility in HCP Mg and BCC Fe," J. Crystal Growth 312, 3238-3242 (2010).

120. N. Pisutha-Arnond, B. Yang, D. H. Lim, **M. Asta** and K. Thornton, "Stability of Strained Thin Films with Interface Misfit Dislocations: A Multiscale Computational Study," Thin Solid Films 519, 809-817 (2010).

121. V. Alexandrov, N. Gronbech-Jensen, A. Navrotsky and **M. Asta**, "First-Principles Computational Study of Defect Clustering in Solid Solutions of ThO_2 with Trivalent Oxides," Phys. Rev. B 82, 174115 (2010).

122. D. L. Olmsted, D. Buta, A. Adland, S. M. Foiles, **M. Asta**, and A. Karma, "Dislocation-Pairing Transitions in Hot Grain Boundaries," Phys. Rev. Lett. 106, 046101 (2011).

123. S. Choudhury, L. Barnard, J. D. Tucker, T. R. Allen, B. Wirth, **M. Asta** and D. Morgan, "Ab-initio based modeling of diffusion in dilute bcc Fe-Ni and Fe-Cr alloys and implications for radiation induced segregation," J. Nucl. Mater. 411, 1-14 (2011).

124. J. P. Palafox-Hernandez, B. B. Laird and **M. Asta**, "Atomistic Characterization of the Cu-Pb Solid-Liquid Interface," Acta Mater. 59, 3137-3144 (2011).

125. Y. Yang, H. Humadi, D. Buta, B.B. Laird, D.Y. Sun, J.J. Hoyt and **M. Asta**, "Atomistic Simulations of Non-Equilibrium Crystal-Growth Kinetics from Alloy Melts," Phys. Rev. Lett. 107, 025505 (2011).

126. V. Radmilovic, C. Ophus, E.A. Marquis, M.D. Rossell, A. Tolley, A. Gautam, **M. Asta** and U. Dahmen, "Highly Monodisperse Core-Shell Particles Created by Solid-State Reactions," Nature Materials 10, 710-715 (2011).

127. B. E. Hanken, C. R. Stanek, N. Gronbech-Jensen and **M. Asta**, "First-Principles Study of the Energetics of Charge and Cation Mixing in $U_{1-x}Ce_xO_2$," Phys. Rev. B 84, 085131 (2011).

128. T. Y. Shvareva, V. Alexandrov, **M. Asta** and A. Navrotsky, "Energetics of Mixing in ThO_2-CeO_2 Fluorite Solid Solutions," J. Nucl. Mater. 419, 72-75 (2011).

129. V. Alexandrov, T. Y. Shvareva, S. Hayun, **M. Asta** and A. Navrotsky, "Actinide Dioxides in Water: Interactions at the Interface," J. Phys. Chem. Lett. 2, 3130-3134 (2011).

130. H. Ding, K. G. Ray, V. Ozolins and **M. Asta**, "Structural and Vibrational Properties of α-MoO_3 from van der Waals Corrected Density Functional Theory Calculations," Phys. Rev. B 85, 012104 (2012).

131. N. Adelstein, J. B. Neaton, **M. Asta** and L. C. De Jonghe, "First-Principles Studies of Proton-Ba Interactions in Doped $LaPO_4$," J. Mater. Chem. 22, 3758-3763 (2012).

132. K. G. Ray, D. Olmsted, N. He, Y. Houndonougbo, B. B. Laird and **M. Asta**, "van der Waals Density Functional Study of CO_2 Binding in Zeolitic Imidazolate Frameworks," Phys. Rev. B 85, 085410 (2012).

133. B. E. Hanken, T. Y. Shvareva, N. Gronbech-Jensen, C. R. Stanek, **M. Asta** and A. Navrotsky, "Energetics of Cation Mixing in Urania-Ceria Solid Solutions with Stoichiometric Oxygen Concentrations," Phys. Chem. Chem. Phys. 14, 5680-5685 (2012).

134. X. Q. Zheng, Y. Yang, Y. F. Gao, J. J. Hoyt, **M. Asta** and D. Y. Sun, "Disorder Trapping During Crystallization of the B2 Ordered NiAl System," Phys. Rev. E 85, 041601 (2012).

135. Y. Yang, D. L. Olmsted, **M. Asta** and B. B. Laird, "Atomistic Characterization of the Chemically Heterogeneous Al-Pb Solid-Liquid Interface," Acta Mater. 60, 4960-4971 (2012).

136. J. A. Aguiar, Q. M. Ramasse, **M. Asta** and N. D. Browning, "Investigating the Electronic Structure of Fluorite-Structured Oxide Compounds: Comparison of Experimental EELS with First-Principles Calculations," J. Phys.: Condens. Matter 29, 295503 (2012).

137. H. Ding, S. Huang, G. Ghosh, P. K. Liaw and **M. Asta**, "A Computational Study of Impurity Diffusivities for 5*d* Transitional Metal Solutes in α-Fe," Scripta Mater. 67, 732-735 (2012).

138. S. J. Fensin, **M. Asta** and R. G. Hoagland, "Temperature Dependence of the Structure and Shear Response of Σ11 Asymmetric Tilt Grain Boundary in Copper from Molecular-Dynamics," Phil Mag. 92, 4320-4333 (2012).

139. T. Radetic, C. Ophus, D. L. Olmsted, **M. Asta** and U. Dahmen, "Mechnism and Dynamics of Shrinking Island Grains in Mazed Bicrystal Thin Films of Au," Acta Mater. 60, 7051-7063 (2012).

140. W. Morris, N. He, K. G. Ray, P. Klonowski, H. Furukawa, I. N. Daniels, Y. A. Houndonougbo, **M. Asta**, B. B. Laird and O. M. Yaghi, "A Combined Experimental-Computational Study of the Effect of Topology on Carbon Dioxide Adsorption in Zeolitic Imidazolate Frameworks," J. Phys. Chem. C 116, 24084-24090 (2012).

141. T. Frolov and **M. Asta**, "Step Free Energies at Faceted Solid-Liquid Interfaces from Equilibrium Molecular Dynamics Simulations," J. Chem. Phys. 137, 214108 (2012).

142. M. de Jong, D. L. Olmsted, A. van de Walle and **M. Asta**, "First-Principles Study of the Structural and Elastic Properties of Rhenium-Based Transition-Metal Alloys," Phys. Rev. B 86, 224101 (2012).

143. C. H. Liebscher, V. Radmilovic, U. Dahmen, **M. Asta** and G. Ghosh, "On the Formation of Hierarchically Structures $L2_1$-Ni_2TiAl Type Precipitates in a Ferritic Alloy," J. Mater. Sci. 48, 2067-2075 (2013).

144. Z. Sun, C. H. Liebscher, S. Huang, Z. Teng, G. Song, G. Wang, **M. Asta**, M. Rawlings, M. E. Fine and P. K. Liaw, "New Design Aspects of Creep-Resistant NiAl-Strengthened Ferritic Alloys," Scripta Mater. 68, 384-388 (2013).

145. A. Adland, A. Karma, R. Spatschek, D. Buta and **M. Asta**, "Phase-Field-Crystal Study of Grain Boundary Premelting and Shearing in BCC Iron," Phys. Rev. B 87, 024110 (2013).

146. Y. Yang, **M. Asta** and B. B. Laird, "Solid-Liquid Interfacial Premelting," Phys. Rev. Lett. 110, 096102 (2013).

147. V. Ozolins, F. Zhou, Y. Liu and **M. Asta**, "Ruthenia-Based Electrochemical Supercapacitors: Insights from First-Principles Calculations," Acc. Chem. Res. 46, 1084-1093 (2013).

148. Y. Houndonougbo, C. Signer, N. He, W. Morris, H. Furukawa, K. G. Ray, D. L. Olmsted, **M. Asta**, B. B. Laird and O. M. Yaghi, "A Combined Experimental-Computational Investigation of Methane Adsorption and Selectivity in a Series of Isoreticular Zeolitic Imidazolate Frameworks," J. Phys. Chem. C 117, 10326-10335 (2013).

149. T. Frolov, D. L. Olmsted, **M. Asta** and Y. Mishin, "Structural Phase Transformations in Metallic Grain Boundaries," Nature Commun. 4:1899 doi: 10.1038/ncomms2919 (2013).

150. C. Ophus, M. K. Santala, **M. Asta** and V. Radmilovic, "Structure and Phase Transitions at a Metal-Ceramic Interface," J. Phys.: Condens. Matter 25, 232202 (2013). *Selected for inclusion in IOPselect*.

151. T. Frolov, S. V. Divinski, **M. Asta** and Y. Mishin, "Effect of Phase Transformations on Diffusion and Segregation in High-Angle Grain Boundaries," Phys. Rev. Lett. 110, 255502 (2013).

152. K. G. Ray, D. L. Olmsted, Y. Houndonougbo, B. B. Laird and **M. Asta**, "Origins of CH_4/CO_2 Adsorption Selectivity in Zeolitic Imidazolate Frameworks: A van der Waals Density Functional Study," J. Phys. Chem. C 117, 14642-14651 (2013).

153. A. van de Walle, P. Tiwary, M. de Jong, D. L. Olmsted, **M. Asta**, A. Dick, D. Shin, Y. Wang, L.-Q. Chen, Z.-K. Liu, "Efficient Stochastic Generation of Special Quasirandom Structures," CALPHAD 42, 13-18 (2013).

154. M. Masin, M. Kotrla, B. Yang, **M. Asta**, M. O. Jahma and T. Ala-Nissila, "Multiscale Modeling of Submonolayer Growth for Fe/Mo(110)," Eur. Phys. J. B 86, 359 (2013).

155. B. E. Hanken, **M. Asta** and W. H. Casey, "Computational Characterization of the Internal Bonding and Solvation Structure for $[Nb_{10}O_{28}]_{aq}^{6-}$," Phys. Chem. Chem. Phys. 15, 20929-20936 (2013).

156. J. M. Solomon, N. Adelstein, L. C. De Jonghe and **M. Asta**, "First Principles Study of Pyrophosphate Defects and Dopant-Defect Interactions in Strontium-Doped Lanthanum Orthophosphate," J. Mater. Chem. A 2, 1047-1053 (2014).

157. V. Alexandrov, N. Gronbech-Jensen, A. Navrotsky and **M. Asta**, "Theoretical Study of Mixing Energetics in Homovalent Fluorite-Structured Oxide Solid Solutions," J. Nucl. Mater. 444, 292-297 (2014).

158. X. Guo, A. H. Tavakoli, S. Sutton, R. K. Kukkadapu, L. Qi, A. Lanzirotti, M. Newville, **M. Asta** and A. Navrotsky, "Cerium Substitution in Yttrium Iron Garnet: Valence State, Structure, and Energetics," Chem. Mater. 26, 1133-1143 (2014).

159. I. M. Markus, N. Adelstein, **M. Asta** and L. C. De Jonghe, "*Ab Initio* Calculation of Proton Transport in $DyPO_4$," J. Phys. Chem. C 118, 5073-5080 (2014).

160. H. Ding, V. I. Razumovsky and **M. Asta**, "Self Diffusion Anomaly in Ferromagnetic Metals: A Density-Functional-Theory Investigation of Magnetically Ordered and Disordered Fe and Co," Acta Mater. 70, 130-136 (2014).

161. F. Lin, I. Markus, D. Nordlund, T.-C. Weng, **M. Asta**, H. Xin and M. Doeff, "Surface Reconstruction and Chemical Evolution of Stoichiometric Layered Cathode Materials for Lithium-Ion Batteries," Nature Commun. 5:3529 doi: 10.1038/ncomms4529 (2014).

162. N. Q. Vo, C. H. Liebscher, M. S. Rawlings, **M. Asta** and D. C. Dunand, "Creep Properties and Microstructure of a Precipitation-Strengthened Ferritic Fe-Al-Ni-Cr Alloy," Acta. Mater. 71, 89-99 (2014).

163. M. B. Alemayehu, G. Mitchson, J. Ditto, B. E. Hanken, **M. Asta** and D. C. Johnson, "Charge Transfer Between PbSe and $NbSe_2$ in $[(PbSe)_{1.14}]_m(NbSe_2)_1$ Ferecrystalline Compounds," Chem. Mater. 26, 1859-1866 (2014).

164. M. J. Kramer, M. I. Mendelev and **M. Asta**, "Structure of Liquid Al and $Al_{67}Mg_{33}$ Alloy: Comparison between Experiment and Simulation," Phil Mag. 94, 1876-1892 (2014).

165. C. Woodward, A. van de Walle, **M. Asta** and D. R. Trinkle, "First-Principles Study of Interfacial Boundaries in Ni-Ni_3Al," Acta Mater. 75, 60-70 (2014).

166. N. Adelstein, J. B. Neaton, **M. Asta** and L. C. De Jonghe, "Density-Functional-Theory Based Calculation of Small Polaron Mobility in Hematite," Phys. Rev. B 89, 245115 (2014).

167. T. Frolov, W. C. Carter and **M. Asta**, "Capillary Instability in Nanowire Geometries," Nano Lett. 14, 3577-3581 (2014).

168. P. Saidi, T. Frolov, J. J. Hoyt and **M. Asta**, "An Angular Embedded Atom Method Interatomic Potential for the Aluminum-Silicon System," Modelling Simul. Mater. Sci. Eng. 22, 055010 (2014).

169. K. G. Ray, D. L. Olmsted, J. Burton, Y. Houndonougbo, B. B. Laird and **M. Asta**, "Gas Membrane Selectivity Enabled by Zeolitic Imidazolate Framework Electrostatics," Chem. Mater. 26, 3976-3985 (2014).

170. H. Ding, H. Lin, B. Sadigh, F. Zhou, V. Ozolins and **M. Asta**, "Computational Investigation of Electron Small Polarons in α-MoO_3," J. Phys. Chem. C 118, 15565-15572 (2014).

171. J. M. Solomon, V. Alexandrov, B. Sadigh, A. Navrotsky and **M. Asta**, "Computational Study of the Energetics and Defect Clustering Tendencies for Y and La-doped UO_2," Acta Mater. 78, 282-289 (2014).

172. J. Aguirre, A. Ferreira, H. Ding, S. A. Jenekhe, N. Kopidakis, **M. Asta**, L. Pilon, Y. Rubin, S. H. Tolbert, B. J. Schwartz, B. Dunn and V. Ozolins, "Panoramic View of Electrochemical Pseudocapacitor and Organic Solar Cell Research in Molecularly Engineered Energy Materials (MEEM)," J. Phys. Chem. C 118, 19505-19523 (2014).

173. M. H. Kumar, S. Dharani, T. Baikie, W. L. Leong, P. P. Boix, R. R. Prabhakar, C. Shi, H. Ding, R. Ramesh, **M. Asta**, M. Graetzel, S. G. Mhaisalkar and N. Mathews,

"Lead-free halide perovskite solar cells with high photocurrents realized through vacancy modulation," Advanced Materials 26, 712-7127 (2014).

174. Z. Wang, Y. Yang, D. L. Olmsted, **M. Asta** and B. B. Laird, "Evaluation of Constant Potential Method in Simulating Electric Double-Layer Capacitors," J. Chem. Phys. 141, 184102 (2014). *Article selected for journal cover*.

175. I. Markus, F. Lin, K. Kam, **M. Asta** and M. Doeff, "Computational and Experimental Investigations of Ti Substitution in $Li_1(Ni_xMn_xCo_{1-x-y}Ti_y)O_2$ for Lithium-Ion Batteries," J. Phys. Chem. Lett. 5, 3649-3655 (2014).

176. C. Toher, J. J. Plata, O. Levy, M. de Jong, **M. Asta**, M. B. Nardelli and S. Curtarolo, "High-Throughput Computational Screening of Thermal Conductivity, Debye Temperature and Gruneisen Parameter Using a Quasiharmonic Debye Model," Phys. Rev. B 90, 174107 (2014).

177. J. M. Solomon, A. Navrotsky and **M. Asta**, "Energetics and Defect Clustering Trends for Trivalent Rare Earth Cations Substituted in UO_2," J. Nucl. Mater. 457, 252-255 (2015).

178. B. Beeler, **M. Asta**, P. Hosemann and N. Gronbech-Jensen, "Effects of Applied Strain on Radiation Damage Generation in Body-Centered Cubic Iron," J. Nucl. Mater. 459, 159-165 (2015).

179. Q. Yu, L. Qi, T. Tsuru, R. Traylor, D. Rugg, J. W. Morris, Jr., **M. Asta**, D. C. Chrzan and A. M. Minor, "Origin of Dramatic Oxygen Solute Strengthening Effect in Titanium," Science 347, 635-639 (2015).

180. B. Medasani, M. Haranczyk, A. Canning and **M. Asta**, "Vacancy Formation Energies in Metals: A Comparison of MetaGGA with LDA and GGA Exchange-Correlation Functionals," Comput. Mater. Sci. 101, 96-107 (2015).

181. M. de Jong, W. Chen, T. Angsten, A. Jain, R. Notestine, A. Gamst, M. Sluiter, C. K. Ande, S. van der Zwaag, J. J. Plata, C. Toher, S. Curtarolo, G. Ceder, K. A. Persson and **M. Asta**, "Charting the Complete Elastic Properties of Inorganic Crystalline Compounds," Scientific Data 2:150009 (2015).

182. H. Ding, B. Medasani, W. Chen, K. Persson, M. Haranczyk, and **M. Asta**, "PyDII: A python framework for computing equilibrium intrinsic point defect concentrations and extrinsic solute site preferences in intermetallic compounds," Computer Physics Communications 193, 118-123 (2015).

183. C. H. Liebscher, V. Radmilovic, U. Dahmen, N. Vo, D. C. Dunand, **M. Asta** and G. Ghosh, "A Hierarchical Microstructure Due to Chemical Ordering in the BCC Lattice: Early Stages of Formation in a Ferritic Fe-Al-Cr-Ni-Ti Alloy," Acta Mater. 92, 220-232 (2015).

184. S. Wolff-Goodrich, B. Hanken, J. Solomon and **M. Asta**, "Special Quasirandom Structure Modeling of Fluorite-Structured Oxide Solid Solutions with Aliovalent Cation Subsitutions," Modelling Simul. Mater. Sci. Eng. 23, 055001 (2015).

185. L. Zhang, J. M. Solomon, **M. Asta** and A. Navrotsky, "A Combined Calorimetric and Computational Study of the Energetics of Rare Earth Substituted UO_2 Systems," Acta Mater. 97, 191-198 (2015).

186. T. Frolov, **M. Asta** and Y. Mishin, "Segregation-Induced Phase Transformations in Grain Boundaries," Phys. Rev. B 92, 020103(R) (2015).

187. P. Palanisamy, M. de Jong, **M. Asta** and J. M. Howe, "Examination of the Electronic Structure of Crystalline and Liquid Al Versus Temperature by In Situ Electron Energy-Loss Spectroscopy (EELS)," Micron 76, 14-18 (2015).

188. M. de Jong, J. Kacher, M. H. F. Sluiter, L. Qi, D. L. Olmsted, A. van de Walle, J. W. Morris, Jr., A. M. Minor and **M. Asta**, "Electronic Origins of Anomalous Twinning in Hexagonal Close Packed Transition Metals," Phys. Rev. Lett. 115, 065501 (2015). *Article selected for journal cover*.

189. C. Ni, H. Ding, **M. Asta** and X. J. Jin, "Computational Study of <1-100> Symmetric Tilt Grain Boundaries in HCP Mg and Ti," Scripta Mater. 109, 94-99 (2015).

190. S. Wolff-Goodrich, F. Lin, I. Markus, D. Nordlund, H. Xin, **M. Asta** and M. Doeff, "Tailoring the Surface Properties of $LiNi_{0.4}Mn_{0.4}Co_{0.2}O_2$ by Titanium Substitution for Improved High Voltage Cycling Performance," Phys. Chem. Chem. Phys. 17, 21778-21781 (2015).

191. H. Zhu, G. Hautier, U. Aydemir, Z. M. Gibbs, G. Li, S. Bajaj, J.-H. Pohls, D. Broberg, W. Chen, A. Jain, M. A. White, **M. Asta**, G. J. Snyder, K. Persson, G. Ceder, "Computational and Experimental Investigation of $TmAgTe_2$ and XYZ_2 Compounds, A New Group of Thermoelectric Materials Identified by First-Principles High-Throughput Screening," J. Mater. Chem. C 3, 10554 (2015).

192. M. de Jong, W. Chen, H. Geerlings, **M. Asta** and K.A. Persson, "A Database to Enable Discovery and Design of Piezoelectric Materials," Scientific Data 2:150053 (2015). *Article featured on journal home page*.

193. K. Niu, T. Frolov, H. L. Xin, J. Wang, **M. Asta** and H. Zheng, "Bubble Nucleation and Migration in a Lead-Iron Hydr(oxide) Core-Shell Nanoparticle," Proc. Natl. Acad. Sci. 112, 12928-12932 (2015).

194. G. Song, Z. Sun, L. Li, X. Xu, M. Rawlings, C. H. Liebscher, B. Clausen, J. Poplawsky, D. N. Leonard, S. Huang, Z. Teng, C. T. Liu, **M. D. Asta**, Y. Gao, D. C. Dunand, M. Chen. M. E. Fine and P. K. Liaw, "Ferritic Alloys with Extreme Creep Resistance via Coherent Hierarchical Precipitates," Sci. Rep. 5, 16327 (2015).

195. T. Krishnamoorthy, H. Ding, C. Yan, W. L. Leong, T. Baikie, Z. Zhang, M. Sherburne, S. Li, **M. Asta**, N. Mathews, and S. B. Mhaisalkar, "Lead-free Germanium Iodide Perovskite Materials for Photovoltaic Application," J. Mater. Chem. A 3, 23829 (2015). *Selected by Editors for "Most popular" anniversary collection of Journal of Materials Chemistry A.*

196. J. Ding, E. Ma, **M. Asta** and R. O. Ritchie, "Second-Nearest-Neighbor Correlations from Connection of Atomic Packing Motifs in Metallic Glasses and Liquids," Sci. Rep. 5, 17429 (2015).

197. W. Chen, J. H. Pohls, G. Hautier, D. Broberg, S. Bajaj, U. Aydemir, Z. M. Gibbs, H. Zhu, **M. Asta**, G. J. Snyder, B. Meredig, M. A. White, K. Persson and A. Jain, "Understanding Thermoelectric Properties from High-Throughput Calculations: Trends, Insights, and Comparisons with Experiment," J. Mater. Chem. C 4, 4414-4426 (2016).

198. Z. Huang, M. D. Abad, J. K. Ramsey, M. Rebelo de Figueiredo, D. Kaoumi, N. Li, **M. Asta**, N. Gronbech-Jensen, and P. Hosemann, "A High Temperature Mechanical Study on PH 13-8 Mo Maraging Steel," Mater. Sci. Eng. A 651, 574-582 (2016).

199. R. Freitas, **M. Asta** and M. de Koning, "Nonequilibrium Free-Energy Calculation of Solids Using LAMMPS," Comp. Mater. Sci. 112, 333-341 (2016). *Selected as "Editor's Choice."*

200. U. Aydemir, J. H. Pohls, H. Zhu, G. Hautier, S. Bajaj, Z. M. Gibbs, W. Chen, G. D. Li, S. Ohno, D. Broberg, S. D. Kang, **M. Asta**, G. Ceder, M. A. White, K. Persson, A. Jain, G. J. Snyder, "$YCuTe_2$: a Member of a New Class of Thermoelectric Materials with $CuTe_4$-based Layered Structure," J. Mater. Chem. A, 4, 2461-2472 (2016).

201. M. de Jong, L. Qi, D. L. Olmsted, A. van de Walle, and **M. Asta**, "Calculations of Planar Defect Energies in Substitutional Alloys Using the Special-Quasirandom-Structure Approach," Phys. Rev. B 93, 094101 (2016). *Selected as "Editor's Suggestion."*

202. X. Guo, E. Tiferet, L. Qi, J. M. Solomon, A. Lanzirotti, M. Newville, M. H. Engelhard, R. K. Kukkadapu, D. Wu, E. S. Ilton, **M. Asta**, S. R. Sutton, H. Xu and A. Navrotsky, "U(V) in Metal Uranates: A Combined Experimental and Theoretical Study of $MgUO_4$, $CrUO_4$ and $FeUO_4$," Dalton Trans. 45, 4622 (2016).

203. J. Ding, **M. Asta** and R. O. Ritchie, "Anomalous Structure-Property Relationships in Metallic Glasses through Pressure-Mediated Glass Formation," Phys. Rev. B 93, 140204 (2016).

204. B. Beeler, **M. Asta**, P. Hosemann, N. Gronbech-Jensen, "Effect of Strain on the Threshold Displacement Energy in Body-Centered Cubic Iron," J. Nucl. Mater. 474, 113-119 (2016).

205. I. M. Markus, S. Engelke, M. Shirpour, **M. Asta** and M. Doeff, "Experimental and Computational Investigation of Lepidocrocite Anodes for Sodium-Ion Batteries," Chem. Mater. 28, 4284-4291 (2016).

206. Z. Wang, D. Olmsted, **M. Asta** and B. B. Laird, "Electric Potential Calculation in Molecular Simulation of Electric Double Layer Capacitors," J. Phys.: Condens. Matter 28, 464006 (2016).

207. T. Frolov, **M. Asta**, Y. Mishin, "Phase Transformations at Interfaces: Observations from Atomistic Modeling," Curr. Opin. Solid State Mater. Sci. 20, 308-315 (2016).

208. G. Xing, H. H. Kumar, W. K. Chong X. Liu, Y. Cai, H. Ding, **M. Asta**, M. Grätzel, S. Mhaisalkar, N. Mathews and T. C. Sum, "Solution-Processed Tin-Based Perovskite for Near Infrared Lasing," Adv. Mater. 28, 8191-8196 (2016).

209. J. C. Agar, S. Pandya, R. Xu, A. K. Yadav, Z. Li, T. Angsten, S. Saremi, **M. Asta**, R. Ramesh and L. W. Martin, "Frontiers in Strain-Engineered Multifunctional Ferroic Materials," MRS Communications 6, 151-166 (2016).

210. M. de Jong, W. Chen, R. Notestine, K. Persson, G. Ceder, A. Jain, **M. Asta** and A. Gamst, "A Statistical Learning Framework for Materials Science: Application to Elastic Moduli of k-nary Inorganic Compounds," Sci. Rep. 6, 34256; doi: 10.1038/srep34256 (2016).

211. B. Medasani, A. Gamst, H. Ding, W. Chen, K. A. Persson, **M. Asta**, A. Canning and M. Haranczyk, "Predicting Defect Behavior in B2 Intermetallics by Merging Ab Initio Modeling and Machine Learning," npj Computational Materials 2, 1 (2016); doi:10.1038/s41524-016-0001-z.

212. J. Ding, Y.-Q. Cheng, H. Sheng, **M. Asta**, R. O. Ritchie and E. Ma, "Universal Structural Parameter to Quantitatively Predict Metallic Glass Properties," Nat. Commun. 7, 13733 doi:10.1038/ncomms13733 (2016).

213. J. M. Solomon, J. Shamblin, M. Lang, A. Navrotsky and **M. Asta**, "Chemical Ordering in Substituted Fluorite Oxides: A Computational Investigation of $Ho_2Zr_2O_7$ and $RE_2Th_2O_7$ (RE=Ho, Y, Gd, Nd, La)," Sci. Rep. 6, 38772 (2016).

214. M. J. S. Rawlings, C. H. Liebscher, **M. Asta** and D. C. Dunand, "Effect of Titanium Additions upon Microstructure and Properties of Precipitation-Strengthened Fe-Ni-Al-Cr Ferritic Alloys," Acta Mater. 128, 103-112 (2017).

215. S. Chakraborty, W. Xie, N. Matthews, M. Sherburne, R. Ahuja, **M. Asta**, S. G. Mhaisalkar, "Rational Design and Combinatorial Screening Approach for Lead-Free and Emergent Hybrid Perovskites," ACS Energy Lett. 2, 837-845 doi:10.1021/acsenergylett.7.b00035 (2017).

216. D. Y. Wan, Y. L. Zhao, Y. Cai, T. C. Asmara, Z. Huang, J. Q. Chen, J. Hong, S. M. Yin, C. T. Nelson, M. R. Motapothula, B. X. Yan, D. Xiang, X. Chi, H. Zheng, W. Chen, R. Xu, Ariando A. Rusydi, A. M. Minor, M. B. H. Breese, M. Sherburne, **M. Asta**, Q-H. Xu, T. Venkatesan, "Electron Transport and Visible Light Absorption in a Plasmonic Photocatalyst based on Strontium Niobate," Nature Comm. 8:15070 (2017).

217. P. Saidi, R. Freitas, T. Frolov, **M. Asta** and J. J. Hoyt, "Free Energy of Steps at Faceted (111) Solid-Liquid Interfaces in the Si-Al System Calculated Using Capillary Fluctuation Method," Comput. Mater. Sci. 134, 184-189 (2017).

218. T. Krishnamoorthy, W. K. Chong, W. Xie, R. Ganguly, S. Muduli, M. Sherburne, **M. Asta**, S. Mhaisalkar, T. C. Sum, H. S. Soo, N. Mathews, "Morphology Independent Stable White-Light Emission from Self-Assembled 2D Perovskites Driven by Strong Exciton-Phonon Coupling to the Organic Framework," Chem. Mater. 29, 3947-3953 (2017).

219. R. Freitas, T. Frolov and **M. Asta**, "Step Free Energies at Faceted Solid Surfaces: Theory and Atomistic Calculations for Steps on the (111) Cu Surface," Phys. Rev. B 95, 155444 (2017).

220. T. C. Asmara, Y. Zhao, M. A. Majidi, C. T. Nelson, M. C. Scott, Y. Cai, D-Y. Wan, D. Schmidt, M. Yang, P. E. Trevisanutto, M. R. Motapothula, M. B. H. Breese, M. Sherburne, **M. Asta**, A. Minor, T. Venkatesan, A. Rusydi, "New Tunable and Low-Loss Correlated Plasmons in Mott-Like Insulating Oxides," Nature Comm. 8, 15271 (2017).

221. T. Angsten, L. W. Martin and **M. Asta**, "Orientation-Dependent Properties of Epitaxially Strained Perovskite Oxide Thin Films: Insights from First-Principles Calculations," Phys. Rev. B 95, 174110 (2017).

222. C. Toher, C. Oses, J. J. Plata, D. Hicks, F. Rose, O. Levy, M. de Jong, **M. Asta**, M. Fornari, M. B. Nardelli, S. Curtarolo, "Combining the AFLOW GIBBS and Elastic Libraries to Efficiently and Robustly Screen Thermomechanical Properties of Solids," Phys. Rev. Materials 1, 015401 (2017).

223. M. de Jong, I. Winter, D. C. Chrzan and **M. Asta**, "Ideal Strength and Ductility in Metals from Second and Third-Order Elastic Constants," Phys. Rev. B 96, 014105 (2017). *Selected as "Editor's Suggestion."*

224. I. S. Winter, M. de Jong, **M. Asta** and D. C. Chrzan, "Computing Elastic Anisotropy to Discover Gum-Metal-Like Structural Alloys," Phys. Rev. Materials 1, 030601(R) (2017).

225. J. Ding, **M. Asta** and R. O. Ritchie, "On the Question of Fractal Packing Structure in Metallic Glasses," Proc. Natl. Acad. Sci. 32, 8458-8463 (2017).

226. T. Radetic, E. Johnson, D. L. Olmsted, Y. Yang, B. B. Laird, **M. Asta** and U. Dahmen, "Step-Controlled Brownian Motion of Nanosized Liquid Pb Inclusions in a Solid Al Matrix," Acta Mater. 141, 427-433 (2017).

227. Y. Cai, W. Xie, H. Ding, Y. Chen, T. Krishnamoorthy, L. Wong, N. Mathews, S. Mhaisalkar, M. Sherburne, **M. Asta**, "Computational Study of Halide Perovskite-Derived A_2BX_6 Inorganic Compounds: Chemical Trends in Electronic Structure and Structural Stability," Chem. Mater. 29, 7740-7749 (2017).

228. A. R. Damodaran, S. Pandya, J. C. Agar, Y. Cao, R. K. Vasudevan, R. Xu, S. Saremi, Q. Li, J. Kim, M. R. McCarter, L. R. Dedon, T. Angsten, N. Balke, S. Jesse, **M. Asta**, S. V. Kalinin, L. W. Martin, Three-State Ferroelastic Switching and Large Electrochemical Responses in $PbTiO_3$ Thin Films," Adv. Mater. 29, 1702069 (2017).

229. J. J Plata, P. Nath, D. Unsanmaz, J. Carrete, C. Toher, M. de Jong, **M. Asta**, M. Fornari, M. Buongiorno Nardelli, S. Curtarolo, "An Efficient and Accurate Framework for Calculating Lattice Thermal Conductivity of Solids: AFLOW-AAPL Automatic Anharmonic Phonon Library," npj Computational Materials 3, 45 (2017); doi:10.1038/s41524-017-0046-7

230. R. Freitas, T. Frolov and **M. Asta**, "Capillary Fluctuations on Surface Steps: An Atomistic Simulation Study for the Model Cu(111) System," Phys. Rev. E 96, 043308 (2017).

231. H. Liang, B. B. Laird, **M. Asta** and Y. Yang, "In-Plane Characterization of Structural and Thermodynamic Properties for the Steps at Faceted Chemically Heterogeneous Solid/Liquid Interfaces," Acta Mater. 143, 329-337 (2017).

232. M. Poschmann, **M. Asta** and D. C. Chrzan, "Convergence of Calculated Dislocation Core Structures in Hexagonal Close Packed Titanium," Modelling Simul. Mater. Sci. Eng. 26, 014003 (2018).

233. D. R. Rittman, C. L Tracy, C.-H. Chen, J. M. Solomon, **M. Asta**, W. L. Mao, S. M. Yalisove and R. C. Ewing, "Phase Transformation Pathways of Ultrafast-Laser-Irradiated Ln_2O_3 (Ln = Er-Lu)," Phys. Rev. B 97, 024104 (2018).

234. T. Angsten and **M. Asta**, "Epitaxial Phase Diagrams of $SrTiO_3$, $CaTiO_3$ and $SrHfO_3$: Computational Investigation Including Role of Antiferrodistortive and A-site Displacement Modes," Phys. Rev. B 97, 134103 (2018).

235. N. Wang, J. Ding, F. Yan, **M. Asta**, R. O. Ritchie, L. Li, "Spatial Correlation of Elastic Heterogeneity Tunes the Deformation Behavior of Metallic Glasses," npj Computational Materials 4:19 (2018).

236. D. Broberg, B. Medasani, N. Zimmermann, G. Yu, A. Canning, M. Haranczyk, **M. Asta** and G. Hautier, "PyCDT: A Python Toolkit for Modeling Point Defects in Semiconductors and Insulators," Computer Physics Communications 226, 165-179 (2018).

237. M. P. Popovic, K. Chen, H. Shen, C. V. Stan, D. L. Olmsted, N. Tamura, **M. Asta**, M. D. Abad and P. Hosemann, "A Study of Deformation and Strain Induced in Bulk by the Oxide Layers Formation on a Fe-Cr-Al Alloy in High-Temperature Liquid Pb-Bi Eutectic," Acta Mater. 151, 301-309 (2018).

238. W. Walukiewicz, I. Rey-Stolle, G. Han, M. Jaquez, D. Broberg, W. Xie, M. Sherburne, N. Mathews and **M. Asta**, "Bistable Amphoteric Native Defect Model of Perovskite Photovoltaics," J. Phys. Chem. Lett. 9, 3878-3885 (2018).

239. J. J. Hoyt, S. Raman, N. Ma and **M. Asta**, "Unusual Temperature Dependence of the Solid-Liquid Interfacial Free Energy in the Cu-Zr System," Comput. Mater. Sci. 154, 303-308 (2018).

240. H. Tan, F. Che, M. Wei, Y. Zhao, M.I. Saidaminov, P. Todorovic, D. Broberg, G. Walters, F. Tan, T. Zhuang, B. Sun, Z. Liang, H. Yuan, E. Fron, J. Kim, Z. Yang, O. Voznyy, **M. Asta** and E.H. Sargent, "Dipolar Cations Confer Defect Tolerance in Wide-Bandgap Metal Halide Perovskites," Nature Comm. 9:3100 (2018).

241. T. Angsten, L. W. Martin and **M. Asta**, "Electronic and Polar Properties of Vanadate Compounds Stabilized by Epitaxial Strain," Chem. Mater. 30, 5870-5877 (2018).

242. J. Ding, Q. Yu, **M. Asta** and R. O. Ritchie, "Tunable Stacking Fault Energies by Tailoring Local Chemical Order in CrCoNi Medium-Entropy Alloys," PNAS 115, 8919-8924 (2018).

243. R. Freitas, R. E. Rudd, **M. Asta** and T. Frolov, "Free Energy of Grain-Boundary Phases: Atomistic Calculations for Σ5(310)[001] Grain Boundary in Cu," Phys. Rev. Mater. 2, 093603 (2018).

244. J. Ding, **M. Asta** and R. O. Ritchie, "Melts of CrCoNi-Based High-Entropy Alloys: Atomic Diffusion and Electronic/Atomic Structure from *ab initio* Simulation," Appl. Phys. Lett. 113, 111902 (2018).

245. L. Ward, A. Dunn, A. Faghaninia, N.E.R. Zimmermann, S. Bajaj, Q. Wang, J. Montoya, J. Chn, K. Bystrom, M. Dylla, K. Chard, **M. Asta**, K.A. Persson, G.J. Snyder, I. Foster, A. Jain, "Matminer: An Open Source Toolkit for Materials Data Mining," Comput. Mater. Sci. 152, 60-69 (2018).

246. M. Hauwiller, X. Zhang, W.-I Liang, C.-H. Chiu, Q. Zhang, W. Zheng, C. Ophus, E.M. Chan, C. Czarnik, M. Pan, F.M. Ross, W.-W. Wu, Y.-H. Chu, P.W. Voorhees, **M. Asta**, A.P. Alivisatos, H. Zheng, "Dynamics of Nanoscale Dendrite Formation in Solution Growth Revealed Through In Situ Liquid Cell Electron Microscopy," Nano Lett. 18, 6427-6433 (2018).

247. R. Freitas, **M. Asta** and V. Bulatov, "Quantum Effects on Dislocation Motion from Ring-Polymer Molecular Dynamics," npj Computational Materials 4:55; doi:10.1038/s41524-018-0112-9 (2018).

248. M. Popovic, D. L. Olmsted, A. M. Bolind, **M. Asta**, S. Sohn, J. Schroers, R. Shao and P. Hosemann, "Investigation of the Effects of Minor Additives to Pb-Bi Eutectic on Interaction with Fe-Cr-Al Alloys at High Temperature: A Study of Pb-Bi-X Liquid Alloys for Heat Transfer Applications," Materials and Design 159, 240-251 (2018).

249. J. Cui, D. L. Olmsted, A. K. Mehta, **M. Asta** and S. E. Hayes, "NMR Crystallography: Evaluation of Hydrogen Positions in Hydromagnesite by 13C{1H} REDOR Solid-State NMR and Density Functional Theory Calculation of Chemical Shielding Tensors," Angew. Chem. Int. Ed. 58, 4210-4216 (2019).

250. M. Poschmann, **M. Asta** and D.C. Chrzan, "Effect of non-Schmid Stresses on <a>-type Screw Dislocation Core Structure and Mobility in Titanium," Comput. Mater. Sci. 161, 261-264 (2019).

251. J. C. Dahl, W. T. Osowiecki, Y. Cai, J. K. Swabeck, Y. Bekenstein, **M. Asta**, E. M. Chan and A. P. Alivisatos, "Probing the Stability of and Bandgaps of $Cs_2AgInCl_6$ and $Cs_2AgSbCl_6$ Lead-Free Perovskite Nanocrystals," Chem. Mater. 31, 3134-3143 (2019).

252. T. C. Pekin, J. Ding, C. Gammer, V. B. Ozdol, C. Ophus, **M. Asta**, R. O. Ritchie and A. M. Minor, "Direct Measurement of Nanostructural Change During In Situ Deformation of a Bulk Metallic Glass," Nature Comm. 10, 2445 (2019).

253. Y. Cai, W. Xie, Y. Teng, P.C. Harikesh, B. Ghosh, P. Huck, K. Persson, N. Mathews, S. Mhaisalkar, M. Sherburne, **M. Asta**, "High-Throughput Computational Study of Halide Double Perovskite Inorganic Compounds," Chem. Mater. 31, 5392-5401 (2019).

254. A. van de Walle, J. Sabisch, A. Minor and **M. Asta**, "Identifying Rhenium Substitute Candidate Multi-Principal-Element Alloys from Electronic Structure and Thermodynamic Criteria," J. Mater. Res. 34, 3296-3304 (2019).

255. W. Zheng, M.R. Hauwiller, W.-I. Liang, C. Ophus, P. Ercius, E.M. Chang, Y.-H. Chu, **M. Asta**, X. Du, A.P. Alivisatos, H. Zheng, "Real Time Imaging of Iron Oxide Spherullite Nanostructure Formation," Nano Research 12, 2889-2893 (2019).

256. J. Lin, H. Chen, Y. Gao, Y. Cai, A. Etman, J. Kang, T. Lei, Z. Lin, L.N. Quan, Q. Kong, M. Sherburne, **M. Asta**, J. Sun, M. F. Toney, J. Wu, P. Yang, "Pressure Induced Semiconductor to Metal Phase Transition of a Charge-Ordered Indium Halide Perovskite," PNAS 116, 23404-23409 (2019).

257. R. Sun, **M. Asta** and A. van de Walle, "First-Principles Thermal Compatibility Between Ru-Based Re-Substitute Alloys and Ir Coatings," Comput. Mater. Sci. 170, 109199 (2019).

258. R. Zhang, S. Zhao, C. Ophus, Y. Deng, S. J. Vachhani, B. Ozdol, R. Traylor, K. C. Bustillo, J.W. Morris, Jr., D.C. Chrzan, **M. Asta**, A.M. Minor, "Direct Imaging of Short-Range Order and Its Relationship to Deformation in Ti-6Al," Sci. Adv. 5, eaax2799 (2019).

259. J. J. Hoyt, S. Raman, P. Saidi and **M. Asta**, "Molecular Dynamics Study of the Thermodynamic and Kinetic Properties of the Solid-Liquid Interface in the Fe-Mn System," Comput. Mater. Sci. 182, 109773 (2020).

260. A. Abu-Odeh, M. Cottura and **M. Asta**, "Insights into Dislocation Climb Efficiency in FCC Metals from Atomistic Simulations," Acta Mater. 193, 172-181 (2020).

261. R. Zhang, S. Zhao, J. Ding, Y. Chong, T. Jia, C. Ophus, **M. Asta**, R. O. Ritchie, A. M. Minor, "Verification of Short-Range Order and Its Impact on the Properties of the CrCoNi Medium Entropy Alloy," Nature 581, 283-287 (2020).

262. B. Febriansyah, C.S. Neo, D. Giovanni, S. Srivastava, Y. Lekina, T. M. Koy, Y. Li, Z. Shen, **M. Asta**, T.C. Sum, N. Mathews, J. England, "Targeted Synthesis of Trimeric Organic-Bromoplumbate Hybrids that Display Intrinsic, Highly Stokes-Shifted, Broadband Emission," Chem. Mater., 32, 4431-4441 (2020).

263. S. Yin, J. Ding, **M. Asta**, R. O. Ritchie, "Ab Initio Modeling of the Energy Landscape for Screw Dislocations in Body-Centered Cubic High-Entropy Alloys," npj Computational Materials 6, 110 (2020).

264. M. E. Manley, K. Hong, P. Yin, S. Chi, Y. Cai, C. Hua, L. L. Daemon, R. P. Hermann, H. Wang, A. May, **M. Asta** and M. Ahmadi, "Giant Isotope Effect on Phonon Dispersion and Thermal Conductivity in Methylammonium Lead Iodide," Sci. Adv. 6, eaaz1842 (2020).

265. I. Vázquez-Fernández, S. Mariotti, O. S. Hutter, M. Birkett, T. D. Veal, T. D. C. Hobson, L. J. Phillips, L. Danos, P. K. Nayak, W. Xie, M. Sherburne, **M. Asta**, K. Durose, "Film Formation and Properties of Cs2TeI6: A New Lead-free Perovskite for Optoelectronics," Chem. Mater. 32, 6676-6684 (2020).

266. H. Liu, **M. Asta**, A. van de Walle, "Computational Assessment of the Efficacy of Oxidation-Resistant Iridium Coatings for Multiple Principal Component Rhenium Substitutes," Scripta Mater. 189, 16-20 (2020).

267. D. L. M. Cordova, S. S. Fender, M. S. Hooshmand, M. Buchanan, J. Davis, T. M. Kam, R. N. Gannon, R. Fischer, P. Lu, B. E. Hanken, **M. Asta**, D. C. Johnson, "The Instability of Monolayer Thick PbSe on VSe2," Chem. Mater. 32, 7992-8003 (2020).

268. Y. Chong, M. Poschmann, R. Zhang, S. Zhao, M. S. Hooshmand, E. Rothchild, D. L. Olmsted, J. W. Morris, Jr., D. C. Chrzan, **M. Asta** and A. M. Minor, "Mechanistic Basis of Oxygen Sensitivity in Titanium," Sci. Adv. 6, eabc4060 (2020).

269. X.-Q. Xu, B. B. Laird, J. J. Hoyt, **M. Asta**, Y. Yang, "Kinetics of Crystallization and Orientational Ordering in Dipolar Particle Systems," Cryst. Growth Des. 20, 7862-7873 (2020).

270. W. Walukiewicz, S. Wang, X. Wu, R. Li, M. P. Sherburne, B. Wu, T. C. Sum, J. W. Ager, **M. Asta**, "The Bright Side and the Dark Side of Hybrid Organic Inorganic Perovskites," J. Phys. Chem. C 124, 27340-27355 (2020).

271. L. Jiang, V. R. Radmilovic, J. E. C. Sabisch, L. Qi, A. M. Minor, D. C. Chrzan, **M. Asta**, "Twin Nucleation From a Single <c+a> Dislocation in Hexagonal Close-Packed Crystals," Acta Mater. 202, 35-41 (2021).

272. Q.-J. Hong, J. Schroers, D. Hofmann, S. Curtarolo, **M. Asta**, A. van de Walle, "Theoretical Prediction of High Melting Temperature for a Mo-Ru-Ta-W HCP Multi-Principal Element Alloy," npj Computational Materials 7, 1 (2021).

273. J. Ding, L. Li, N. Wang, L. Tian, **M. Asta**, R.O. Ritchie, T. Egami, "Universal Nature of the Saddle States of Structural Excitations in Metallic Glasses," Materials Today Physics 17, 100359 (2021).

274. Y. Yang, S. Y. Yang, B. Xiang, S. Yin, T. C. Pekin, X. Li, R. Zhang, K. Yano, **M. Asta**, C. Grigoropoulos, F. I. Allen, A. M. Minor, "Evaluating the Effects of Pillar Shape and Gallium Ion Beam Damage on the Mechanical Properties of Single Crystal Aluminum Nano-Pillars," J. Mater. Res. (2021). https://doi.org/10.1557/s43578-021-00125-5

275. W. Walukiewicz, S. Wang, X. Wu, M. P. Sherburne, J. W. Ager, **M. Asta**, "Photophysics of Localized Deep Defect States in Hybrid Organic-Inorganic Perovskites," J. Phys. Chem. C 125, 6975-6982 (2021).

276. F. Walsh, **M. Asta**, R. O. Ritchie, "Magnetically Driven Short-Range Order Can Explain Anomalous Measurements in CrCoNi," PNAS 118, e2020540118 (2021).

277. S. Zhao, R. Zhang, Y. Chong, X. Li, A. Abu-Odeh, E. Rothchild, D. C. Chrzan, **M. Asta**, J.W. Morris, Jr., A. M. Minor, "Defect Reconfiguration in a Ti-Al Alloy via Electroplasticity," Nat. Mater. 20, 468-472 (2021).

278. A. Ben-Moshe, A. da Silva, A. Muller, A. Abu-Odeh, P. Harrison, J. Waelder, F. Niroui, C. Ophus, A. M. Minor, **M. Asta**, W. Theis, P. Ercius, A. P. Alivisatos, "The Chain of Chirality Transfer in Tellerium Nanocrystals," Science 372, 729-733 (2021).

279. N. Winner, H. Williams, R. Scarlat, and **M. Asta**, "Ab-Initio Simulation Studies of Cr Solvation in Fluoride Molten Salts," Journal of Molecular Liquids 335, 116351 (2021).

280. T. Frolov, D. L. Medlin, **M. Asta**, "Dislocation Content of Grain Boundary Phase Junctions and Its Relation to Grain Boundary Excess Properties," Phys. Rev. B 103, 184108 (2021).

281. S. Yin, Y. Zuo, A. Abu-Odeh, H. Zheng, X.-G. Li, J. Ding, S. P. Ong, **M. Asta**, R. O. Ritchie, "Atomistic Simulations of Dislocation Mobility in Refractory High-Entropy Alloys and the Effect of Chemical Short-Range-Order," Nature Comm. 12, 4873 (2021).

282. Y. Chong, R. Zhang, M. S. Hooshmand, S. Zhao, D. C. Chrzan, **M. Asta**, J. W. Morris, Jr., A. M. Minor, "Elimination of oxygen sensitivity in α-titanium by substitutional alloys with Al," Nature Comm. 12, 6158 (2021).

283. M. C. Folgueras, J. Jin, M. Gao, L. N. Quan, J. A. Steele, S. Srivastava, M. B. Ross, R. Zhang, F. Seeler, K. Schierle-Arndt, **M. Asta**, P. Yang, "Lattice Dynamics and Optoelectronic Properties of Vacancy-Ordered Double Perovskite Cs_2TeX_6 ($X=Cl^-$, Br^-, I^-) Single Crystals," J. Phys. Chem. C, 125, 45, 25126-25139 (2021).

284. B. P. Uberuaga, P. Simonnin, K. M. Rosso, D. K. Schreiber, **M. Asta**, "The Effect of Cr Alloying on Defect Migration at Ni Grain Boundaries," J. Mater. Sci. 57, 10499-10516 (2022).

285. M. Poschmann, I. S. Winter, **M. Asta**, D. C. Chrzan, "Molecular Dynamics Studies of <a>-type Screw Dislocation Core Structure Polymorphism within Hexagonal Close Packed Metals," Phys. Rev. Mater. 6, 013603 (2022).

286. D. C. Chrzan, M. Poschmann, I. S. Winter and **M. Asta**, "Thermodynamic Model for Polymorphic Dislocation Core Spreading within Hexagonal Close Packed Metals," Phys. Rev. Mater. 6, 013604 (2022).

287. A. Abu-Odeh, D. L. Olmsted, **M. Asta**, "Screw Dislocation Mobility in a Face-Centered Cubic Solid Solution with Short-Range Order," Scripta Mater. 210, 114465 (2022).

288. A. Abu-Odeh and **M. Asta**, "Modeling the Effect of Short-Range Order on Cross-Slip in an FCC Solid Solution," Acta Mater. 226, 117615 (2022).

289. E. Chen, A. Tamm, T. Wang, M. E. Epler, **M. Asta** and T. Frolov, "Modeling Antiphase Boundary Energies of Ni_3Al-Based Alloys Using Automated Density Functional Theory and Machine Learning," npj Computational Materials 8, 1-10 (2022).

290. J. Yan, S. Yin, **M. Asta**, R. O. Ritchie, J. Ding, Q. Yu, "Anomalous Size Effect on Yield Strength Enabled by Compositional Heterogeneity in High-Entropy Alloy Nanoparticles," Nature Comm. 13, 1-8 (2022).

291. F. Walsh, **M. Asta** and L. W. Wang, "Realistic magnetic thermodynamics by local quantization of a semiclassical Heisenberg model", npj Computational Materials 8, 186 (2022).

292. B. Zhang, **M. Asta** and L. W. Wang, "Machine Learning force field for Fe-H system and investigation of Role of hydrogen on the crack propagation in α-Fe," Comput. Mater. Sci. 214, 111709 (2022).

293. L. Langford, N. Winner, A. Hwang, H. Williams, L. Vergari, R. Scarlat, **M. Asta**, "Constant-Potential Molecular Dynamics Simulations of Molten-Salt Double Layers in FLiBe and FLiNaK," J. Chem. Phys. 157, 094705 (2022).

294. E. Rothchild, M. Poschmann, **M. Asta**, D. C. Chrzan, "Dislocation Glide Driven Interstitial Shuffling of Oxygen Interstitials in Titanium," Phys. Rev. M 6, 093601 (2022).

295. E. Chen and **M. Asta**, "Using Juypyter Tools to Design an Interactive Textbook to Guide Undergraduate Research in Materials Informatics," J. Chem. Educ. 99, 3601-3606 (2022).

296. M. Acharya, H. Ling, D. Lou, M. Ramesh, B. Hanrahan, G. Velarde, **M. Asta**, K. Persson and L. W. Martin, "Exploring the Morphotropic Phase Boundary in Epitaxial $PbHf_{1-x}Ti_xO_3$ Thin Films," Chem. Mater. 34, 9613-9623 (2022).

297. M. Zhang, Q. Yu, C. Frey, F. Walsh, M. I. Payne, P. Kumar, D. Liu, T. M. Pollock, **M. D. Asta**, R. O. Ritchie, A. M. Minor, "Determination of Peak Ordering in CrCoNi Medium-Entropy Alloy via Nanoindentation," Acta Mater. 241, 118380 (2022).

298. A. Abu-Odeh, T. Allaparti and **M. Asta**, "Structure and Glide of Lomer and Lomer-Cottrell Dislocations: Atomistic Simulations for Model Concentrated Alloy Solid Solutions," Phys. Rev. Materials 6, 103603 (2022).

299. F. Walsh, R. O. Ritchie and **M. Asta**, "Theoretical Antiferromagnetism of Ordered Face-Centered-Cubic Cr-Ni Alloys," Phys. Rev. Materials 6, 113602 (2022).

300. D. Liu, Q. Yu, S. Kabra, M. Jiang, P. Forna-Kreutzer, R. Zhang, M. Payne, F. Walsh, B. Gludovatz, **M. Asta**, A. M. Minor, E. P. George, R. O. Ritchie, "Exceptional Fracture Toughness of CrCoNi-Based Medium- and High-Entropy Alloys at 20 Kelvin," Science 378, 978-983 (2022).

301. J. Cui, T. R. Prisk, D. L. Olmsted, V. Su, **M. Asta**, S. E. Hayes, "Resolving the Chemical Formula on Nesquehonite via NMR Crystallography, DFT Computation and Complementary Neutron Diffraction," Chem. Eur. J. e202203052 (2022).

302. Y. Yang W. Zhou, S. Yin, S. Y. Wang, Q. Yu, M. J. Olszta, Y.-Q. Zhang, S. E. Zeltmann, M. Li, M. Jin, D. K. Schreiber, J. Ciston, M. C. Scott, J. R. Scully, R. O. Ritchie, **M. Asta**, J. Li, M. P. Short, A. M. Minor, "One Dimensional Wormhole Corrosion in Metals," Nature Comm. 14, 988 (2023).

303. A. Ferrari, F. Kormann, **M. Asta** and J. Neugebauer, "Simulating Short-Range Order in Compositionally Complex Materials," Nature Computational Science 3, 221-229 (2023).

304. Z. Pei, S. Zhao, M. Detrois, P. Jablonski, J. Hawk, D. Alman, **M. Asta**, A. Minor, and M. Gao, "Theory-Guided Design of High-Entropy Alloys with Enhanced Strength-Ductility Synergy," Nature. Comm. 14, 2519 (2023).

305. D. Broberg, K. Bystrom, S. Srivastava, D. Dahliah, B.A.D. Williamson, L. Weston, D.O. Scanlon, G-M. Rignanese, S. Dwaraknath, J. Varley, K. Persson, **M. Asta**, G. Hautier, "High-Throughput Calculations of Charged Point Defect Properties with Semi-Local Density Functional Theory – Performance Benchmarks for Materials Screening Applications," npj Computational Materials 9, 72 (2023).

306. A. Banerjee, E. Holby, A. Kohnert, S. Srivastava, **M. Asta**, B.P. Uberuaga, "Thermokinetics of Point Defects in alpha-Fe_2O_3," Electron. Struct. 5, 024007 (2023).

307. N. Bieberdorf, **M. Asta** and L. Capolungo, "Grain Boundary Effects in High-Temperature Liquid-Metal Dealloying: A Multi-Phase Field Study," npj Computational Materials 9, 127 (2023).

308. A. Abu-Odeh, B.P. Uberuaga, **M. Asta**, "Barrier-Free Predictions of Short-Range Ordering/Clustering Kinetics in Binary FCC Solid Solutions," Acta Mater. 257, 119185 (2023).

309. F. Walsh, M. Zhang, R.O. Ritchie, A.M. Minor, **M. Asta**, "Extra Electron Reflections Do Not Necessitate Short-Range Order," Nature Mater. 22, 926-929 (2023).

310. S. Srivastava, B.P. Uberuaga, **M. Asta**, "Density Functional Theory Study of Local Environment Effects on Oxygen Vacancy Properties in Magnetite," J. Phys. Chem. C 127, 17460-17472 (2023).

311. R. Woods-Robinson, Y. Xiong, J.-X. Shen, N. Winner, M.K. Horton, **M. Asta**, A.M. Ganose, G. Hautier, K.A. Persson, "Designing Transparent Conductors Using Forbidden Optical Transitions," Matter 6, 3021-3039 (2023).

312. J. Wan, Q. Zhang, J. Liang, K. Bustillo, Z. Al Balushi, **M. Asta**, H. Zheng, "Visualizing Facets Asymmetry Induced Directional Movement of Cadmium Chloride Nanomotor," Nano Lett. 23, 10132-10139 (2023).

313. P.P.P.O. Borges, R.O. Ritchie, **M. Asta**, "Local Lattice Distortions and the Structural Instabilities in BCC Nb-Ta-Ti-Hf High-Entropy Alloys: An Ab Initio Computational Study," Acta Mater. 262, 119415 (2024).

314. N.-J. Liu, Z.-J. Wang, J. Ding, **M. Asta**, R.O. Ritchie, B. Gan, E. Ma, Z.-W. Shan, "The Origin of the High Propensity for Nanoscale Deformation Twins in the CrCoNi Medium-Entropy Alloy," J. Mater. Sci. & Tech. 181, 63-71 (2024).

315. B. Zhang, Z. Zhang, K. Xun, **M. Asta**, J. Ding, E. Ma, "Minimizing the Diffusivity Difference between Vacancies and Interstitials in Multi-Principal Element Alloys," PNAS (accepted).

316. W. Wang, F. Walsh, R.O. Ritchie, **M. Asta**, "Elucidating the Roles of Chemistry, Compositional Complexity, and Short-Range Order in Dislocation Energetics of Body-Centered-Cubic Concentrated Solid Solutions," Phys. Rev. Mater. (accepted).

317. S.H. Mills, R.D. Hayes, N. Bieberdorf, S.E. Zeltmann, A.M. Kennedy, L. Capolungo, **M. Asta**, R.O. Scarlat, A.M. Minor, "Elucidating the Role of Cr Migration in Ni-Cr Exposed to Molten FLiNaK via Multiscale Characterization," Acta Mater. (submitted).

318. M. S. Hooshmand, R. Zhang, Y. Chong, E. Chen, T. Frolov, D. L. Olmsted, A. M. Minor, **M. Asta**, "Twin-Boundary Structural Phase Transitions in Elemental Titanium," Nature Mater. (submitted); arXiv:2103.06194.

Non-Refereed Journals, Conference Proceedings, Book Chapters

1. G. Ceder, **M. Asta**, and D. de Fontaine, "Oxygen Ordering in $YBa_2Cu_3O_Z$ at Low Temperature," Mat. Res. Soc. Symp. Proc., Vol. 169, pp. 189-194 (1990).
2. D. de Fontaine, **M. Asta**, C. Wolverton, and H. Dreyssé, "CVM Approach to Alloy Theory," Joint Research Report, Monbusho International Scientific Research Program sponsored by Japanese Ministry of Education, Science and Culture, 1990.
3. **M. Asta**, M. Sluiter, Prabhakar P. Singh, D. de Fontaine, T. Hong, and A.J. Freeman, "First Principles Study of Phase Stability in the Al-Ti System," Mat. Res. Soc. Symp. Proc., Vol. 186, pp. 33-40 (1991).
4. Prabhakar P. Singh, **M. Asta**, D. de Fontaine, and M. Van Schilfgaarde, "Ground State Properties of the Al-Ti System," Mat. Res. Soc. Symp. Proc., Vol. 186, pp. 41-46 (1991).
5. D. de Fontaine, G. Ceder, **M. Asta**, and R. McCormack, "Oxygen Ordering and Superconductivity in $YBa_2Cu_3O_X$," in High Temperature Superconducting Compounds III: Processing and Microstructure Property Relationships, S. H. Wang, A. DasGupta and E. Collings, eds., TMS, pp. 411-418 (1991).
6. D. de Fontaine, **M. Asta**, C. Wolverton and H. Dreyssé, "First-Principles Calculations of Phase Diagrams," Proc. of JIMIS-6, Sendai, Japan, pp. 199-207 (1991).
7. **M. Asta**, D. de Fontaine, M. van Schilfgaarde, M. Sluiter and M. Methfessel, "A First-Principles Study of the Phase Stability of fcc-Based Ti-Al Alloys," Mat. Res. Soc. Symp. Proc., Vol. 278, pp. 313-318 (1992).
8. **M. Asta**, R. McCormack, M. van Schilfgaarde, G. Ceder, and D. de Fontaine, "Phase Stability of fcc- and hcp-based Intermetallics: The Ti-Al and Cd-Mg Systems," Statics and Dynamics of Alloy Phase Transformations, ed. by P. E. A. Turchi and A. Gonis, Plenum, New York, pp. 581-584 (1992).
9. D. de Fontaine, G. Ceder, **M. Asta**, and R. McCormack, "Energetics and Statistics of Order in Alloys with Application to Oxide Superconductors," in Ordering and Disordering in Alloys, A. R. Yavari, ed., Elsevier, pp. 372-384 (1992).
10. **M. Asta**, M. van Schilfgaarde, and D. de Fontaine, "A First-Principles Study of the Phase Stability of fcc- and hcp-based Ti-Al Alloys," Mat. Res. Soc. Symp. Proc., Vol. 288, pp. 153-158 (1993).
11. R. McCormack, **M. Asta**, D. de Fontaine, and G. Ceder, "The hcp Ising Model in the Cluster Variation Approximation," Mat. Res. Soc. Symp. Proc., Vol. 291, pp. 395-400 (1993).
12. **M. Asta**, R. McCormack, and D. de Fontaine, "Phase Stability in the Cd-Mg System," in Alloy Modelling and Design, ed. by G. M. Stocks and P. E. A. Turchi, TMS, pp. 121-126 (1993).
13. **M. Asta**, A. Ormeci, J. W. Wills, and R. C. Albers, "First-Principles Study of Phase Stability in the Ternary Ti-Al-Nb Alloy System," Mat. Res. Soc. Symp. Proc., Vol. 364, pp. 157-162 (1995).

14. **M. Asta**, "Thermodynamic Properties of Coherent Interphase Boundaries in FCC Substitutional Alloys," in Theory and Applications of the Cluster Variation and Path Probability Methods, edited by J. L. Moran-Lopez and J. M. Sanchez (Plenum, New York, 1996), pp. 237-254.

15. **M. Asta**, "Thermodynamic Properties of Coherent Interphase Boundaries in Substitutional FCC Alloys," Mat. Res. Soc. Symp. Proc., Vol. 398, pp. 281-286 (1996).

16. M. Sluiter, **M. Asta** and Y. Kawazoe, "Prediction of Matrix-Precipitate Interfacial Free Energies: Application to Al-Al_3Li," Science Reports of the Research Institutes of Tohuku University Vol. 41, 97 (1996).

17. Cathy Lane Rohrer, **M. Asta**, Stephen M. Foiles, and Robert W. Hyland, Jr., "A Kinetic Model of Precipitate Evolution," Mat. Res. Soc. Symp. Proc., Vol. 398, pp. 477-482 (1996).

18. **M. Asta**, V. Ozolins and C. Woodward, "First Principles Approach to Modeling Alloy Phase Equilibria," JOM Vol. 53, pp. 16-19 (2001).

19. **M. Asta**, D. Y. Sun and J. J. Hoyt, "Role of Atomic-Scale Simulation in the Modeling of Solidification Microstructure," in Thermodynamics, Microstructures and Plasticity, vol. 108 of *NATO Science Series II. Mathematics, Physics and Chemistry*, edited by A. Finel, D. Maziere and M. Veron (Kluwer Academic Publishers, Boston, 2003), pp. 411-425.

20. J. J. Hoyt, A. Karma, **M. Asta**, and D. Y. Sun, "From Atoms to Dendrites," JOM Vol. 56, pp. 49-54 (2004).

21. J. J. Hoyt, **M. Asta**, T. Haxhimali, A. Karma, R. E. Napolitano, R. Trivedi, B. B. Laird and J. R. Morris, "Crystal-Melt Interfaces and Solidification Morphologies in Metals and Alloys," MRS Bulletin Vol. 29, pp. 935-939 (2004).

22. **M. Asta**, F. Spaepen and F. van der Veen, "Solid-Liquid Interfaces: Molecular Structure, Thermodynamics and Crystallization," MRS Bulletin Vol. 29, pp. 920-922 (2004).

23. A. van de Walle and **M. Asta**, "First-Principles Modeling of Phase Equilibria," Handbook of Materials Modeling, edited by S. Yip (Springer, New York, 2005), article 1.16.

24. G. Ghosh, A. van de Walle and **M. Asta**, "First-Principles Phase Stability Calculations of $L1_2$, $D0_{22}$, and $D0_{23}$ Structures in Al-TM (=Ti,Zr,Hf)-Zn Systems," Proceedings of Solid ->Solid Phase Transformations in Inorganic Materials 2005, edited by J. M. Howe, D. E. Laughlin, J. K. Lee, U. Dahmen and W. A. Soffa (TMS, Warrendale, PA, 2005), pp. 651-656.

25. Kathleen Stair, Jefferson Z. Liu and **Mark Asta**, "Ultra-Sonic Measurement and Computation of Elastic Constants," Proceedings of the 2006 American Society for Engineering Education (ASEE) Conference, available on-line (2006).

26. **Mark Asta**, Dallas R. Trinkle and Christopher Woodward, "Ab-Initio Molecular Dynamics Simulations of Molten Ni-Based Superalloys," Proceedings of the 2006

High Performance Computing User's Group Conference (IEEE Computing Society, Los Alamitos, CA 2007), pg. 177-181.

27. A. van de Walle, G. Ghosh and **M. Asta**, "Ab Initio Modeling of Alloy Phase Stability," Applied Computational Materials Modeling: Theory, Simulation and Experiment, edited by G. Bozzolo, R. D. Noebe and P. Abel, pages 1-34 (Springer, New York, 2007).

28. **Mark Asta**, Susan M. Kauzlarich, Kai Liu, Alexandra Navrotsky and Frank E. Osterloh, "Inorganic Nanoparticles – Unique Properties and Novel Applications," Material Matters, vol. 2, pages 3-6 (2007).

29. **Mark Asta**, Dallas R. Trinkle and Christopher Woodward, "Ab-Initio Molecular Dynamics Simulations of Molten Ni-Based Superalloys," Proceedings of the HPCMP User's Group Conference 2007 (IEEE Computing Society, Los Alamitos, CA 2007), pp. 147-152.

30. **C**hristopher Woodward, **Mark Asta**, Dallas R. Trinkle and Stefano Angioletti-Uberti, "Ab-Initio Molecular Dynamics Simulations of Molten Ni-Based Superalloys," Proceedings of the HPCMP User's Group Conference 2008 (IEEE Computing Society, Los Alamitos, CA 2008), pp. 169-174.

31. Katsuyo Thornton, Samanthule Nola, R. Edwin Garcia, **Mark Asta**, and G. B. Olson, "Computational Materials Science and Engineering Education: A Survey of Trends and Needs," JOM, vol. 61, No. 10, pp. 12-17 (2009).

32. J. J. Hoyt, **M. Asta** and A. Karma, "Atomistic Simulations of Solute Trapping and Solute Drag," in Solidification of Containerless Undercooled Melts, First Edition, edited by D. M. Herlach and D. M. Matson, pages 363-380 (Wiley-VCH Verlag GmbH & Co, 2012).

33. I. M. Markus, N. Adelstein, **M. Asta** and L. C. De Jonghe, "Ab Intio Calculation of the Energy Landscape for Protons in $DyPO_4$," ECS Trans. 45, 111-115 (2012) (doi:10.1149/1.3701298).

34. J. Solomon, N. Adelstein, **M. Asta** and L. C. De Jonghe, "Charge-Compensating Pyrophosphate Defect Structures in Sr-doped $LaPO_4$," ECS Trans. 45, 117-120 (2012) (doi:10.1149/1.3701299).

35. C. Woodward, J. Lill, **M. Asta** and D. R. Trinkle, "Molecular-Dynamics Simulations of Ni-Based Superalloys," in Superalloys 2012, edited by E. S. Huron, R. C. Reed, M. C. Hardy, M. J. Mills, R. E. Montero, P. D. Portella and J. Telesman (Wiley-VCH Verlag GmbH & Co, 2012), DOI: 10.1002/9781118516430.ch59.

36. **M. Asta**, "Computational Materials Discovery and Design," JOM 66, 364-365 (2014).

37. P. E. A. Turchi and **M. Asta**, "Summary Report of CALPHAD XLI – Berkeley, California, USA, 2012," CALPHAD 45, 204-250 (2014).

38. M. Popovic, Y. Yang A. M. Bolind, V. B. Ozdol, D. L. Olmsted, **M. Asta** and P. Hosemann, "Transmission Electron Microscopy (TEM) Study of the Oxide Layers

Formed on Fe-12Cr-4Al Ferritic Alloy in an Oxygenated Pb-Bi Environment at 800 C," JOM 70, 1471-1477 (2018).

39. R. A. Enrique, **M. Asta** and K. Thornton, "Computational Materials Science and Engineering Education: An Updated Survey of Trends and Needs," JOM 70, 1644-1651 (2018).
40. A. van de Walle and **M. Asta**, "High Throughput Calculations in the Context of Alloy Design," MRS Bulletin 44, 252-256 (2019).
41. A. Navrotsky, K. Lilova, D. Wu, **M. Asta**, "Thermodynamics of Complex Solids," J. Mater. Res. 34, 3241-3242 (2019).
42. C. Guneau, B. Sundman, **M. Asta**, "Computational Thermodynamics: Applications to Nuclear Materials," in Comprehensive Nuclear Materials, 2nd Edition, edited by R. Konings and R. Stoller (Elsevier, 2020).
43. E. Chen, **M. Asta**, A. Minor, "Integrating Programming-Based Modules into a Materials Characterization Laboratory Course to Reinforce Data Science and Scientific Writing," 2023 ASEE Annual Conference & Exposition (2023).
44. F. Walsh, A. Abu-Odeh and **M. Asta**, "Reconsidering Short-Range Order in 3d Complex Concentrated Alloys," MRS Bulletin 48, 753-761 (2023).

PROFESSIONAL ACTIVITIES

Co-organizer of International Workshops, Symposia, Summer Schools, Short Courses

1. International Workshop: "*Structural and Thermodynamic Properties of Alloy Materials,*" Aruba (1999)
2. Materials Research Society: "*Structure and Dynamics of Defects and Interfaces: Predicting the Evolution of Phase and Defect Microstructures*," Boston, MA, November, 2000
3. TMS Annual Meeting: "*Computational Modeling of Phase Transformations*," Seattle, WA, February, 2002
4. American Association for Crystal Growth and Epitaxy (ACCGE) Annual Meeting Symposium: "*Atomic-Scale Simulations of Crystal Growth from the Melt*," Seattle, WA, August, 2002.
5. TMS Annual Meeting: "*Computational Methods in Materials Education*," San Diego, CA, March, 2003.
6. Centre Européen de Calcul Atomique et Moléculaire (CECAM) Workshop: "*Crystal-Melt Interfaces: Structure, Thermodynamics and Growth*," Lyon, France, June 23-25, 2003.
7. TMS Annual Meeting: "*The Didier de Fontaine Symposium on the Thermodynamics of Alloys*," Charlotte, NC, March 14-18, 2004.
8. Materials Research Society: "*Modeling of Morphological Evolution at Surfaces and Interfaces*," Boston, MA, November 30 – December 2, 2004.

9. TMS Annual Meeting: "*Computational Thermodynamics and Phase Transformations Symposium*," Orlando, FL, February 25–March 1, 2007.
10. PSI-K Network Workshop: "*Multiscale Approach to Alloys: Advances and Challenges*," Sigtuna, Sweden, June 16-19, 2007.
11. Member of the International Advisory Committee for the Electron Microscopy and Multiscale Modeling 2007 (EMM07) conference, Moscow, Russia, September 17-21, 2007.
12. Deutschen Physikalischen Gesellschaft (DFG) Meeting Symposium: "*Modern Developments in Multiphysics Materials Simulations*," Berlin, Germany, February 28-29, 2008.
13. APS March Meeting: "*Frontiers of Computational Materials*," New Orleans, LA, March 10, 2008.
14. Materials Science & Technology (MS&T) Meeting: "*Phase Stability, Diffusion Kinetics and Their Applications*," Pittsburgh, PA, October 6-8, 2008.
15. TMS Annual Meeting: "*Advanced Characterization and Modeling of Phase Transformations in Metals in Honor of David N. Seidman on his 70th Birthday*," San Francisco, CA, February 16-18, 2009.
16. Co-Leader of Dynamics panel and co-author of final report for the DOE workshop on Discovery in Basic Energy Sciences: The Role of Computing at the Extreme Scale, August 13-15, 2009, Bethesda, MD.
17. Materials Research Society: "*Multiphysics Modeling in Materials Design*," Boston, MA, November 30 – December 4, 2009.
18. TMS Annual Meeting: "*Hume Rothery Symposium: Configurational Thermodynamics of Materials*," Seattle, WA, February 14 – 18, 2010.
19. Electron Microscopy and Multi-Scale Modeling (EMMM11) Conference, Tahoe City, CA, May 22-27, 2011.
20. Chair of Physical Metallurgy Gordon Conference, Stonehill College, Easton, MA, July 31 – August 5, 2011.
21. TMS Annual Meeting: "*Computational Thermodynamics and Kinetics*," Orlando, FL, March 12-15, 2012.
22. CALPHAD XLI Meeting, Berkeley, CA, June 3-8, 2012.
23. Harnessing the Materials Genome: Accelerated Materials Development via Computational and Experimental Tools, Vail, CO, September 30 – October 5, 2012.
24. Co-Organizer of two short courses held in conjunction with TMS meetings: Introduction to Computational Materials Science and Engineering Tools Short Course, July 11-12, 2013, Salt Lake City, UT; Integrated Computational Materials Education Short Course, March 4, 2011, Orlando, FL.
25. TMS Annual Meeting: "*Hume-Rothery Award Symposium: Multicomponent Alloy Metallurgy, the Bridge from Materials Science to Materials Engineering*," Orlando, FL, March 16-19, 2015.

26. TMS Annual Meeting: "*Micromechanics of Structurally Inhomogeneous Materials: An FMD Symposium in Honor of Armen Khachaturyan*," Orlando, FL, March 16-19, 2015.

27. 9th Pacific Rim International Conference on Advanced Materials and Processing (PRICM9): "*Modelling and Simulation of Microstructures and Processing*," Kyoto, Japan, August 2-5, 2016.

28. Co-Organizer of Integrated Computational Materials Education Summer School, University of Michigan, July 18-29, 2011; University of Michigan, June 11-22, 2012; University of California, Santa Barbara, June 14-25, 2014; University of Michigan, June 15-26; University of California, Berkeley, June 6-17, 2016; University of Michigan, June 5-16, 2017; University of Michigan, June 4-15, 2018.

29. Co-Organizer of National Science Foundation Emerging Opportunities and Research Infrastructure Needs in Metals Research workshop, June, 2021.

Review Panels and Advisory Boards

1. Member of the *National Resource Allocations Committee* (NRAC) and the *Partnership Resource Allocations Committee* (PRAC) of the National Science Foundation's *Partnership for Advanced Computational Infrastructure* (PACI) (March 2002-June 2005).

2. Member of Peer Review Panel: Department of Energy, Office of Basic Energy Science, Division of Materials Science, Review Panel for Oak Ridge National Laboratory, June 2-5, 2002, and January 17-19, 2006.

3. Member of Review Panel: National Science Foundation Review Panel for the Nanoscale Interdisciplinary Research Teams (NIRT), February 24, 2004.

4. Member of the Committee of Visitors (COV) for the Materials Sciences and Engineering Programs in the Office of Basic Energy Sciences of the U. S. Department of Energy, April 3-5, 2006.

5. Member of the Scientific Advisory Board, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany, 2007 – 2013.

6. External Reviewer, UCLA Academic Senate Program Review, Department of Materials Science and Engineering, April 9-10, 2007.

7. Member of Review Panel: Los Alamos National Laboratory Materials Capability Review, May 15-18, 2007; April 29 – May 1, 2008.

8. Member of UC Davis Mathematics Graduate Program Review Committee, University of California, Davis, March 12-13, 2009.

9. Review of NNSA Project "First principles modeling of microscopic scintillation mechanisms using a Many-Body Green's function approach," Lawrence Livermore National Laboratory, Livermore, CA, March 7, 2011.

10. Member of the External Advisory Board for the Materials Research Laboratory (MRL) at the University of Illinois, Urbana-Champaign, 2013 – 2015.

11. Member of International Scientific Committee, Solid-Solid Phase Transformations in Inorganic Materials (PTM 2015) Conference, Whistler, BC, Canada, June 28 – July 3, 2015.
12. Member of external review committee for the Department of Chemical Engineering and Materials Science at the University of Minnesota, Minneapolis, MN, October 20-21, 2015.
13. Member of external review committee for the Department of Materials Science and Engineering at the University of Michigan, Ann Arbor, MI, December 12-14, 2016.
14. Review of NNSA Project "Advanced Materials for Detectors," Lawrence Berkeley National Laboratory, Berkeley, CA, May 18-19, 2016.
15. Chair of external review committee for the Department of Materials Science and Engineering at the University of Illinois, Urbana-Champaign, IL, February 20-21, 2017.
16. Member of the Lawrence Livermore National Security LLC (LLNS) Science and Technology Committee, 2015 – present.
17. Member of the Los Alamos National Security LLC (LANS) Science and Technology Committee, 2015-2018.
18. Member of the External Advisory Board for the Materials Research Science and Engineering Center on Structured Interfaces at the University of Wisconsin, Madison, 2013 – 2017.
19. Member of external review committee for the Department of Metallurgical and Materials Engineering, Colorado School of Mines, Golden, CO, November 9-10, 2017; September 8-9, 2022.
20. Member of the Materials Advisory Board, Department of Chemical and Materials Engineering, University of Kentucky, October, 2017 – 2023.
21. Member of Triennial Review Committee for the Oak Ridge National Laboratory Department of Energy, Office of Basic Energy Sciences, Materials Science and Engineering Programs, Oak Ridge, TN, April 24-6, 2018.
22. Invited participant, Alternative Materials Workshop (virtual), hosted by the Information Technology and Innovation Foundation, Boston University Institute for Sustainable Energy, and the Fraunhofer USA Center for Manufacturing Innovation, as part of a workshop series on "Widening the Lens on Innovation for Clean Manufacturing." February 17, 2021.
23. Invited Participant, NSF Convergence Accelerator Workshop on "Accelerating Translational Materials R&D for Global Challenges." May 20 - June 30, 2021.
24. Member of Department of Energy Vehicle Technologies Office Annual Merit Review, Materials Technologies R&D Panel (Virtual Review), June 21-24, 2021; June 20-23, 2022.

25. Member of the External Advisory Board for the Data and Informatics Graduate Intern-Traineeship: Materials at the Atomic Scale (DIGI-MAT) at the University of Illinois, Urbana-Champaign, June, 2021 – present.
26. Member of the External Advisory Board, Department of Materials Science & Engineering, University of Wisconsin, August, 2021 – present.
27. Member of the External Review Team for the Northwestern-Argonne Institute of Science and Engineering (NAISE) at Northwestern University, April 13-15, 2022.
28. Member of the Physical & Computational Sciences Directorate Advisory Committee, Pacific Northwest National Laboratory (PNNL), Richland, WA, July, 2023 – present.
29. Member of Review Panel and External Reviewer for National Science Foundation Review of 2023 Materials Research Science & Engineering Center proposals.

Editorial Boards and Guest Editor

1. Member of Editorial Board for Interface Science (June, 2002-December, 2004).
2. "Key Reader" Member of the Board of Review for Metallurgical and Materials Transactions (2000 - 2012).
3. Member of Editorial Board for CALPHAD (2004 – present).
4. Guest editor (together with F. Spaepen and F. van der Veen) of MRS Bulletin issue on "Solid-Liquid Interfaces: Structure, Thermodynamics and Crystallization," December, 2004.
5. Guest editor for *Thermodynamics of Complex Solids* issue of the Journal of Materials Research (Volume 34, Issue 19, October 14, 2019).

Professional Society Committees

1. TMS, Education Committee (2001-2004).
2. TMS, Physics and Chemistry of Materials Committee (1999-present); Vice Chair (2011 – 2013); Chair (2013 – 2015); Former Chair (2015-2017).
3. TMS, Information Technology Committee (2008-2010).
4. TMS, Integrated Computational Materials Engineering Committee (2009-present).
5. TMS, Awards Committee (2012 – 2015).
6. APS, Nominating Committee for Division of Materials Physics (2013 – 2014).
7. University Materials Council: Member 2013-2017; Executive Committee Member 2013-2017; Chair: 2015-2016.
8. APS, Fellowship Committee for Division of Materials Physics (2018 – 2019).

Journal and Proposal Reviews

1. Referee of manuscripts for Physical Review B, Physical Review Letters, Physical Review X, Journal of Chemical Physics, Modelling and Simulation in Materials Science and Engineering, CALPHAD, Science, Nature, Nature Communications, Acta Materialia, PNAS, and Surface Science.

2. Referee of proposals for the National Science Foundation, the Department of Energy, and the Petroleum Research Fund.

INVITED LECTURES, TUTORIALS AND PANELS

1. National Institute of Standards and Technology, Joint Metallurgy/Ceramics Division Seminar, December 1992; Gaithersburg, MD; "First-Principles Studies of Phase Stability: Applications to Oxygen Ordering in $YBa_2Cu_3O_Z$ and the Ti-Al Phase Diagram".
2. Sandia National Laboratories, Computational Materials Science Department Seminar, June 1993; Livermore, CA; "First-Principles Calculations of Alloy Phase Diagrams".
3. Los Alamos National Laboratory, Center for Materials Science Seminar, July 1993; Los Alamos, NM; "First-Principles Studies of Alloy Phase Stability".
4. Materials Science Department Seminar, University of California at Berkeley, October 20, 1994; "Thermodynamic Properties of Coherent Precipitates: A First-Principles Study of Guinier-Preston Zones in Al-Ag."
5. International Workshop on the Theory and Applications of the Cluster and Path Probability Methods, San Juan, Teotihuacan, Mexico, June 18-22, 1995; "Thermodynamic Properties of Coherent Interphase Boundaries in fcc Substitutional Alloys."
6. Universidad Nacional Autonoma de Mexico, Chemistry Department Seminar, June 23, 1995; Mexico City, Mexico; "Thermodynamic Properties of Coherent Interphase Boundaries in fcc Substitutional Alloys."
7. The Fall TMS Meeting, Cleveland, OH, October 29-November 2, 1995; "First-Principles Studies of the Structure and Stability of Multicomponent Alloy Phases: Application to the Ti-Al-Nb System."
8. 8.CECAM Workshop on Theoretical Predictions of Alloy Phase Stability, Lyon, France, June 10-14, 1996; "Thermodynamic Properties of Interphase and Antiphase Boundaries in Substitutional Alloys."
9. Physics Department at University of Barcelona, Barcelona, Spain, June 19, 1996; "First-Principles Calculations of Alloy Thermodynamic Properties."
10. Materials Science Department Seminar, University of California at Berkeley, November 14, 1996; "Thermodynamic Properties of Alloy Interfaces and Multilayers."
11. Calphad XXVI Meeting, Palm Coast, FL, May 11-16, 1997; "First-Principles Calculations of Alloy Phase Diagrams."
12. The Fall TMS Meeting, Indianapolis, IN, September 15, 1997; "First-Principles Study of Site Occupations in Ti-Al-Nb *B*2 Alloys."
13. The Spring TMS Meeting, San Antonio, TX, February 17, 1998, "First-Principles Studies of the Thermodynamic Properties of Interphase and Antiphase Boundaries in Substitutional Alloys."

14. The Naval Research Laboratory, Washington, D.C., May 15, 1998, "First-Principles Calculations of Thermodynamic Properties for Alloy Interfaces."
15. The Ohio State University, Columbus, Ohio, October 29, 1998, "First-Principles Calculations of Structural and Thermodynamic Properties of Metallic Alloys."
16. Northwestern University, Evanston, Illinois, April 29, 1999, "Alloy Formation in Ultrathin Metallic Films."
17. Air Force Research Laboratory, Dayton, Ohio, December 7, 1999, "First-Principles Study of Bulk and Defect Properties in Al-Sc Based Alloys."
18. National Institute of Standards and Technology, Gaithersburg, Maryland, June 22, 2000, "First-Principles Calculations of Phase Boundaries in Dilute Alloys Including Ionic Vibrational Free Energy."
19. Computational Materials Science Network Workshop, Santa Fe, New Mexico, January 11, 2001, "Equilibrium Properties of Solid-Liquid Interfaces in Alloys."
20. The Annual TMS Meeting, New Orleans, LA, February 12, 2001, "First Principles Studies of Phase Stability and Short-Range Order in HCP Alloys."
21. University of Kentucky, Department of Chemical Engineering and Materials Science/Center for Computational Science Colloquium, February 21, 2001, "Bridging Length Scales in the Modeling of Materials Structure."
22. The Computational Materials Science Workshop, Sponsored by AMPTIAC on behalf Dr. Lewis Sloter, Staff Specialist, Materials & Structures, Office of the Deputy Undersecretary of Defense, April 24, 2001, "Hierarchical Multiscale Approaches for Computational Modeling of Phase Transformations."
23. Ford Research Center, March 17, 2001, "Atomic-Scale Modeling of Liquids and Solid-Liquid Interfaces in Alloys."
24. Sixth U.S. National Congress on Computational Mechanics, August 1, 2001, "Atomic-Scale Modeling of Phase Transformations in Alloys."
25. Laboratoire L2MP, Universite d'Aix-Marseille III, September 7, 2001, "Atomic-Scale Modeling of Solid-Liquid Interfaces in Alloys."
26. Workshop on Thermodynamic and Structural Properties of Materials, September 13, 2001, "Atomic-Scale Modeling of Solid-Liquid Interfaces and Phase-Equilibria in Alloys."
27. Computational Materials Science Network Workshop, Northeastern University, Boston, MA, September 24, 2001, "Solid-Liquid Interfacial Thermodynamic Properties in Alloys."
28. Materials Research Society, Boston, MA, November 28, 2001, "Atomic-Scale Modeling of Heterophase Interfaces in Alloys."
29. Nanoparticles in Materials Science, Franco-American Workshop, Northwestern University, December 3, 2001, "Nano-scale Composition Modulation in Ultrathin Alloy Films."

30. Computational Materials Science Network Workshop, National Institute of Standards and Technology, Gaithersburg, MD, March 26, 2002, "Atomic-Scale Modeling of Solid-Liquid Interfaces in Alloys."

31. Kansas University, Department of Chemistry Colloquium, April 12, 2002, "Computational Modeling of Structure Development Accompanying Phase Transformations."

32. CIMTEC Forum on New Materials, Florence, Italy, July 15, 2002, "Thermodynamic Properties of Bulk Metallic Alloys Studied by First-Principles Methods."

33. Max-Planck Institute, Stuttgart, Germany, July 19, 2002, "First-Principles Studies of Nanometer-Scale Compositionally Modulated Structures in Ultrathin Films of Bulk-Immiscible Alloys."

34. Lecturer at NATO-Advanced-Study Institute on "Thermodynamics, Microstructure and Plasticity," held in Frejus, France, September 2-13, 2002. Title of three lectures: "Role of Atomic-Scale Simulations in the Modeling of Microsctructure."

35. Computational Materials Science Network Workshop, Ames Laboratory, October 16, 2002, "Solid-Liquid Interface Kinetic Coefficient from Atomic-Scale Simulations."

36. The Annual TMS Meeting, San Diego, CA, March 3, 2003, "First-Principles Studies of Phase Partitioning and Interfacial Segregation."

37. The Annual TMS Meeting, San Diego, CA, March 4, 2003, "Atomic-Scale Simulations of Alloy Solid-Liquid Interfaces."

38. Computational Materials Science Network Workshop, University of California at San Diego, San Diego, CA, March 6, 2003, "Solid-Liquid Interfaces in BCC Fe."

39. Harvard University, Materials Science Seminar, May 8, 2003, "Nanometer-Scale Phase Separation in Ultrathin Alloy Films."

40. CALPHAD XXXII, La Malbaie, Quebec, Canada, May 26, 2003, "First-Principles Calculations of Alloy Phase Diagrams: Towards Automation and Integration with CALPHAD."

41. CECAM Workshop on Crystal-Melt Interfaces: Structure Thermodynamics and Growth, June 23, 2003, "Solid-Liquid Interfacial Free Energies from Molecular Dynamics Simulations of Capillary Fluctuations."

42. Max-Planck Institute, Stuttgart, Germany, June 27, 2003, "First-Principles Modeling of Surface Alloys and Alloy Interfaces."

43. ACCGE-15, Keystone Colorado, July 22, 2003, "Thermodynamic and Kinetic Properties of Solid-Liquid Interfaces in Metals and Alloys by Atomic-Scale Simulations."

44. Computational Materials Science Network Workshop, Colorado School of Mines, Golden, CO, October 2, 2003, "Solid-Liquid Interfacial Free Energies in Metals: FCC vs. BCC."

45. 2003 Lawrence Symposium on Critical Issues in Epitaxy, Arizona State University, Tempe, AZ, October 10, 2003, "Nanometer-Scale Composition Modulation in Ultrathin Alloy Films."

46. University of Wisconsin, Materials Science Colloquium, December 11, 2003, "First-Principles Computational Thermodynamics in the Study of Nanostructured Alloys."

47. American Physical Society, 2004 March Meeting, Montreal, Canada, March 24, 2004, "Segregation at Coherent Interphase Boundaries: The Case of Mg at Al/Al_3Sc."

48. Johns Hopkins University, Colloquium, Department of Materials Science and Engineering, April 7, 2004, "Nanometer-Scale Compositionally Modulated Structures in Ultrathin Alloy Films."

49. University of California at Davis, May 10, 2004, "Multiscale Modeling of Crystal Growth From the Melt: From Atoms to Dendrites."

50. Seagate Research, Pittsburgh, PA, June 9, 2004, "Atomic-Scale Computational Modeling of Alloy Nanostructures: Phase Stability and Interfacial Effects."

51. ASME Nano Training Bootcamp, June 29, 2004, "Introduction to Statistical Mechanics (and Computer Simulation)."

52. The Annual TMS Meeting, San Francisco, CA, February 15, 2005, "Energetics of Ge/Si(100) Island Formation: Role of Strain-Dependent Surface Energies."

53. The Annual TMS Meeting, San Francisco, CA, February 15, 2005, "Crystal-Melt Interfacial Energies in Metals: Role of Crystal Structure."

54. ACCGE-15, Keystone Colorado, July 15, 2005, "Steps on Faceted Crystal-Melt Interfaces: Atomic-Scale Computer Simulations."

55. International Materials Research Congress 2005, Cancun, Mexico, August 24, 2005, "Surface Stress in Nanostructures."

56. Workshop on Modeling Materials in Extreme Environments (ME2), September 24, 2005, Washington D. C., "Computationally Assisted Design of Nb-Based Structural Alloys for High-Temperature Applications."

57. Materials Science & Technology Conference, 2005, September 26, 2005, Pittsburgh, PA, "Atomic-Scale Simulations of the Properties of Rough and Faceted Crystal-Melt Interfaces."

58. 7th Annual Warren Symposium, January 23, 2006, Ringberg Castle, Germany, "Order Disorder Transitions in Alloy Nanoparticles."

59. Materials Science Seminar, January 26, 2006, Max Planck Institute, Stuttgart, Germany, "Multiscale Modeling of Nanostructures in Heteroepitaxial Systems."

60. Materials Science Seminar, January 31, 2006, RWTH, Aachen, Germany, "Atomic-Scale Simulations of Crystal-Melt Interfaces for Multiscale Modeling of Solidification Microstructure."

61. Materials Science Seminar, February 1, 2006, Max Planck Institute, Duesseldorf, Germany, "Nano-scale Precipitation in Al-Sc and Fe-Cu Alloys: Insights from First-Principles Calculations."

62. Ab-Initio Description of Iron and Steel (ADIS-2006) Workshop, February 20, 2006, Ringberg Castle, Germany, "Atomic-Scale Simulations of Crystal-Melt Interfaces for Multiscale Modeling of Solidification Microstructure."

63. Fritz-Haber Institute Seminar, Feburary 27, 2006, Berlin, Germany, "The Forces That Stabilize Nanoscale Surface Structures – Insights from Atomic-Scale Simulations."

64. University of the Pacific, Department of Chemistry Seminar, March 7, 2006, Stockton, CA, "Multiscale Modeling of Materials – From Atoms to Complex Nano and Microstructures."

65. American Physical Society March Meeting, March 13, 2006, Baltimore, MD, "Multiscale Modeling of Solidification Microstructures – Atomic-Scale Simulations of Crystal-Melt Interfaces and Beyond."

66. TMS Annual Meeting, March 14, 2006, San Antonio, TX, "Properties of Steps at Faceted Crystal-Melt Interfaces from Molecular-Dynamics Simulations."

67. TMS Annual Meeting, March 14, 2006, San Antonio, TX, "Application of First-Principles Methods in the Modeling of Multicomponent Alloys."

68. UCLA, Department of Materials Science and Engineering Colloquium, May 19, 2006, Los Angeles, CA, "Nanostructures from Heteroepitaxial Growth: Insights from Multiscale Calculations."

69. Multiscale Modeling of Materials: Mathematics and Computation, Workshop Sponsored by the Northwest Consortium for Multiscale Mathematics and Applicants, May 29, 2006, Tacoma, WA, "Atomic-Scale Simulations of Crystal-Melt Interfaces for Multiscale Modeling of Solidification Microstructures."

70. 2006 Electronic Structure Workshop, The Ohio State University, June 25, 2006, Columbus, OH, "Ab-Initio Alloy Thermodynamics."

71. Sandia National Laboratores, July 6, 2006, Albuquerque, NM, "Nanostructures from Heteroepitaxial Growth: Insights from Modeling at Multiple Scales."

72. Physical Metallurgy Gordon Research Conference, July 25, 2006, Holderness School, New Hampshire, "Modeling of Solid-Liquid Interface Properties and Their Role in Determining Solidification Microstructures."

73. International Materials Research Congress 2006, Cancun, Mexico, August 21, 2006, "Ab-Initio Molecular Dynamics Simulations of Molten Super-Alloys."

74. Material Physics Department Seminar, Sandia National Laboratories, Livermore, CA, August 29, 2006, "Properties of Steps at Faceted Crystal-Melt Interfaces from Molecular-Dynamics Simulations."

75. Trivedi Symposium: Critical Issues and Future Directions in Solidification Science, Ames, IA, September 19, 2006, "Atomic-Scale Modeling of Crystal-Melt Interfaces in Metals and Alloys."

76. Surface and Interface Science at the Atomic Scale: DOE-BES Contractors Meeting, Airlie Conference Center, VA, October 31, 2006, "Computational Investigations of Crystal-Melt Interfaces in Metals and Alloys."

77. Materials Research Society, Boston, MA, November 29, 2006, "Properties of Alloy Crystal-Melt Interfaces from Atomistic Simulations."

78. Materials Science Department Colloquium, University of Michigan, Ann Arbor, Michigan, February 10, 2007, "Modeling the Crystal-Melt Interface."

79. UC Berkeley, Department of Materials Science and Engineering Colloquium, March 22, 2007, Berkeley, CA, "Nanostructures from Heteroepitaxial Growth: Insights from Modeling at Multiple Scales."

80. Lawrence Livermore National Laboratory, Livermore, California, April 3, 2007, "The Crystal-Melt Interface: Insights from Atomic-Scale Modeling."

81. Department of Materials Science and Engineering Colloquium, Massachusetts Institute of Technology, Cambridge, MA, May 4, 2007, "The Crystal-Melt Interface: Insights from Atomic-Scale Modeling."

82. Multiscale Approach to Alloys: Advances and Challenges, Sigtuna, Sweden, June 19, 2007, "Nanometer-Scale Phase Separation in Epitaxial Alloy Films."

83. Diffraction Club Seminar, Max Planck Institute, Stuttgart, Germany, July 13, 2007, "First-Principles Modeling of Nanometer-Scale Phase Separation in Ultrathin Epitaxial Alloy Films."

84. MS&T'07, Detroit, Michigan, September 17, 2007, "Ab-Initio Molecular Dynamics Simulations of Molten Superalloys."

85. MS&T'07, Detroit, Michigan, September 17, 2007, "Models for Teaching Materials Modeling."

86. Materials Modelling Laboratory Seminar, Oxford University, Oxford, UK, October 16, 2007, "Ab-Initio Molecular Dynamics: Applications to Structure and Thermodynamic Properties of Molten Superalloys and NiTi."

87. Department of Materials Science Colloquium, Oxford University, Oxford, UK, October 18, 2007, "First-Principles Modeling of Nanoscale Precipitation Strengthened Alloys."

88. Asian-Pacific Conference on Computational Mechanics '07, Kyoto, Japan, December 3, 2007, "Energetics of Stranski-Krastanov Growth from Hybrid First-Principles and Continuum Scale Modeling."

89. National Center for Electron Microscopy, Berkeley, CA, January 24, 2008, "First-Principles Modeling of Nano-scale Precipitation Strengthened Al Alloys."

90. Los Alamos National Laboratory, MST-8 Seminar, Feburary 22, 2008, "The Crystal-Melt Interface – Insights from Atomic-Scale Modeling."

91. NIST Diffusion Workshop, Gaithersburg, MD, May 12, 2008, "Diffusion of Substitutional Impurities in BCC Fe – First-Principles Modeling."

92. International Workshop on Interfaces, Santiago de Compostela, Spain, June 23, 2008, "The Crystal-Melt Interface: Insights from Atomic-Scale Modeling."

93. Gordon Research Conference: High Temperature Materials, Processes & Diagnostics, Colby College, Main, July 23, 2008, "Ab-Initio Modeling of Molten Super-Alloys: Structure, Thermodynamics and Diffusivities from Quantum Molecular-Dynamics Simulations."

94. MS&T '08, Pittsburgh, PA, October 6, 2008, "Applications of First-Principles Thermodynamics and Kinetics in the Context of Materials Optimization."

95. Materials Research Society, Boston, MA, December 3, 2008, "Computational Approaches to UO_2 Defects and Radiation Damage."

96. ICAMS Seminar, Interdisciplinary Centre for Advanced Materials Simulation, Ruhr University Bochum, Germany, February 9, 2009, "Ab-Initio Modeling of Molten Alloys."

97. TMS Annual Meeting, February 16, 2009, San Francisco, CA, "Molecular Dynamics Investigations of Faceted Growth at the Nanoscale."

98. TMS Annual Meeting, February 16, 2009, San Francisco, CA, "Effects of Substrate Symmetry and Prepatterning on the Stability of Compositional Patterns in Ultrathin Alloy Films."

99. TMS Annual Meeting, February 18, 2009, San Francisco, CA, "Status of Computational Materials Education in the US: Results of Recent Surveys."

100. Princeton Institute for the Science and Technology of Materials (PRISM) Colloquium, March 25, 2009, Princeton University, "Nanoscale Size Effects in Faceted Crystal Growth: Insights from Molecular Dynamics Simulations."

101. High-Temperature Capillarity – 2009 (HTC-2009), May 8, 2009, Athens, Greece, "Crystal-Melt Interfaces: Insights from Atomistic Simulations."

102. PICS 2009 Workshop, June 11, 2009, Marseilles, France, "Faceted Solid-Liquid Interfaces: Insights on Structure, Dynamics and Size Effects from Molecular Dynamics Simulations."

103. ES09 Workshop, June 25, 2009, University of California, Davis, "Ab-Initio Molecular Dynamics Modeling of Molten Superalloys."

104. Bridging the Gap Workshop, October 15, 2009, McMaster University, Hamilton, Ontario, Canada, "Calculation of Substitutional Impurity Diffusivities in α-Fe Using First-Principles Methods."

105. International Symposium on Defects, Transport and Related Phenomena, MS&T '09 Meeting, Pittsburg, PA, October 28, 2009, "First-Principles Studies of Defect Chemistry in UO_2."

106. "Nanoscale Computational Materials Science" Tutorial, TMS Annual Meeting, Seattle, WA, February 14, 2010.

107. Symposium on Heterogeneous Nucleation and Initial Microstructure Evolution in Alloys and Compounds, TMS Annual Meeting, Seattle, WA, February 15, 2010,

"Molecular Dynamics Simulation of Two-Dimensional Nucleation in the Context of Crystal Growth."

108. Materials Modeling Seminar, University of British Columbia, Vancouver, Canada, March 10, 2010, "Ab-Initio Calculations in Alloy Design."

109. Materials Research Society, San Francisco, CA, April 8, 2010, "Computational Modeling of Oxide Solid Solutions for Nuclear Energy."

110. SIAM Symposium on Thermodynamics and Kinetics of Materials Interfaces: Advances and Challenges in Theory and Modeling, Philadelphia, PA, May 24, 2010, "Dynamics of Faceted Solid-Liquid Interfaces Probed by Atomistic Simulations."

111. PTM 2010: Solid-Solid Phase Transformations in Inorganic Materials, Avignon, France, June 8, 2010, "Molecular Dynamics Simulations of Solute Trapping and Solute Drag."

112. PICS 2010 Workshop, June 15, 2010, Marseilles, France, "Molecular Dynamics Simulations of Hot Grain Boundaries."

113. Thomas Young Centre Highlight Seminar, Imperial College London, June 21, 2010, "Crystal-Melt Interfaces: Insights from Atomic-Scale Simulations."

114. Lecturer for three-hour "Master Course" at the Thomas Young Centre, Imperial College London, June 24, 2010. Title of course: "First-Principles Modeling of Configurational Thermodynamics in Crystalline Alloys & Compounds."

115. Lecturer at Summer School on Computational Materials Science, Miramar Palace, San Sebastian, Spain, June 29, 2010. Title of lecture: "First-Principles Modeling of Configurational Thermodynamics in Crystalline Alloys & Compounds: Cluster Expansions & Related Methods."

116. International Materials Research Congress 2010, Cancun, Mexico, August 18, 2010, "First-Principles Modeling of Fluorite Solid Solutions Relevant to Nuclear Fuels."

117. Ψ_k Conference 2010, Berlin, Germany, September 14, 2010, "First-Principles Modeling of Urania and Thoria Solid Solutions."

118. NIST Workshop on Wires, Whiskers and Walls: Energy Applications at the Nanoscale, September 30, 2010, "Nucleation Kinetics at a Faceted Solid-Liquid Interface."

119. National Energy Technology Laboratory, MSEFE Weekly Seminar, Albany, Oregon, November 9, 2010, "First-Principles Modeling in Alloy Design."

120. Pennsylvania State University, Department of Materials Science and Engineering Colloqium, State College, PA, December 9, 2010, "Thermochemical Properties of Nuclear Fuels: Insights from First-Principles Calculations."

121. Fudan University, Department of Physics Seminar, Shanghai, China, January 7, 2011, "Thermochemical Properties of Nuclear Fuels: Insights from First-Principles Calculations."

122. East China Normal University, Department of Physics Seminar, Shanghai, China, January 7, 2011, "Thermochemical Properties of Nuclear Fuels: Insights from First-Principles Calculations."

123. Shanghai Jiao Tong University, Department of Materials Science and Engineering, Shanghai, China, January 10, 2011, "Crystal-Melt Interfaces: Insights from Atomic-Scale Modeling."

124. ISIJ Special Lecture, University of Tokyo, Tokyo, Japan, January 12, 2011, "Physical Property Estimation Based on the Atomistic Approach, which Relates to Solidification and Microstructure Formation."

125. Frontiers in Solidification Science Symposium, TMS Annual Meeting, San Diego, CA, February 28, 2011, "Molecular Dynamics Simulations of Alloy Rapid Solidification."

126. Computational Thermodynamics and Kinetics Symposium, TMS Annual Meeting, San Diego, CA, March 1, 2011, "Mixing Properties in Oxide Solid Solutions Relevant to Nuclear Fuels."

127. Approaches for Investigating Phase Transformations at the Atomic Scale Symposium, TMS Annual Meeting, San Diego, CA, March 1, 2011, "Computational and Experimental Investigations of Core-Shell Precipitates in Al-Sc-Li Alloys."

128. Lyman Handy Colloquium Seminar, Department of Chemical Engineering and Materials Science, University of Southern California, March 10, 2011, "Crystal-Melt Interfaces: Insights from Atomic-Scale Modeling."

129. Materials Research Society, San Francisco, CA, April 28, 2011, "Structural Disordering & Phase Transitions in Hot Grain Boundaries: Insights from Molecular Dynamics & Phase-Field Crystal Simulations."

130. European Materials Research Society, Nice, France, May 9, 2011, "Insights into the Structure of High-Temperature Grain Boundaries from Atomistic Simulations."

131. Energy Frontiers Research Centers Summit, Washington, DC, May 26, 2011, "Computational Modeling of Actinide Compounds: From Clusters to Complex Crystal Structures."

132. Quantitative Micro-Nano (QMN-2) Approach to Predicting SCC of Fe-Cr-Ni Alloys – Initiation of SCC, Sun Valley, Idaho, June 15, 2011, "Grain Boundaries at High Homologous Temperatures Studied by Atomistic Simulations."

133. 2nd Annual U.S. Department of Energy Nuclear Energy Programs Materials Science and Engineering Materials Cross-cut Workshop, and The 5th Annual Asia-Pacific Nuclear Energy Forum on Materials for Nuclear Applications, Berkeley, CA, June 23, 2011, "DOE EFRC Materials Science of Actinides: Experimental and Computational Studies of Energetics."

134. Lawrence Livermore National Laboratory Computational Chemistry and Materials Science Summer Institute, Livermore, CA, June 27-28, 2011, "Materials Interfaces Studied by Atomistic Simulations."

135. Interfaces, Grain Boundaries and Surfaces from Atomistic and Macroscopic Approaches – Fundamental and Engineering Issues Symposium, MS&T11 Conference, Columbus, OH, October 17, 2011, "Atomistic Modeling of Chemically Heterogeneous Solid-Liquid Interfaces."

136. Phase Stability, Diffusion, Kinetics and Their Applications (PSDK-VI) Symposium, Session Honoring John W. Cahn, Recipient of ASM's 2011 J. Willard Gibbs Phase Equilibria Award, MS&T11 Conference, Columbus, OH, October 18, 2011, "Coherent Precipitation in Ternary Al Alloys: Insights from First-Principles Modeling."

137. Materials Research Lecture, California Institute of Technology, Pasadena, CA, November 30, 2011, "Highly Monodisperse Core-Shell Particles Created by Solid-State Reactions in Alloys."

138. Materials Science and Engineering Colloquium, Northwestern University, Evanston, IL, January 17, 2012, "Highly Monodisperse Core-Shell Particles Created by Solid-State Reactions in Alloys."

139. American Physical Society March Meeting, Focus Session on Frontiers in Computational Thermodynamics of Materials, Boston, MA, February 28, 2012, "Thermodynamic Stability of Actinide-Dioxide Solid Solutions and Surface Interactions with Water."

140. Solid-State Interfaces II: Toward an Atomistic-Scale Understanding of Structure, Properties, and Behavior through Theory and Experiment, TMS Annual Meeting, Orlando, FL, March 15, 2012, "Shrinking Island Grains: Mobilities and Driving Forces."

141. Symposium on Hard Coatings and Vapor Deposition Technology – Computational Design and Experimental Development of Functional Thin Films, International Conference on Metallurgical Coatings & Thin Films, San Diego, CA, April 24, 2012, "Molecular Dynamics Studies of Grain Boundaries in Mazed-bicrystal Thin Films."

142. Fundamentals of Thermodynamic Modelling of Materials Summer School, INSTN – CEA, Saclay, France, July 6, 2012, "Modelling Liquids from First Principles."

143. ICAMS Seminar, Bochum, Germany, July 10, 2012, "Dynamics of Grain-Boundary Motion Studied by In-Situ Electron Microscopy and Molecular Dynamics Simulations."

144. Max-Planck-Institut für Eisenforschung Seminar, Düsseldorf, Germany, July 19, 2012, "Dynamics of Grain-Boundary Motion Studied by In-Situ Electron Microscopy and Molecular Dynamics Simulations."

145. Foundations of Molecular Modeling and Simulation, Mt. Hood, OR, July 26, 2012, "Selective Gas Adsorption in Zeolitic Imidazolate Frameworks: Insights from Molecular Modeling and van der Waals Density Functional Theory Calculations."

146. Institute of Pure and Applied Mathematics Workshop on Atomistics and Mesoscale Modeling of Materials Defects, University of California, Los Angeles, October 23, 2012, "Insights into Grain-Boundary Motion through Coupling of In-Situ Electron Microscopy and Molecular Dynamics Simulations."

147. Hume-Rothery Award Symposium, TMS Annual Meeting, San Antonio, TX, March 4, 2013, "First-Principles Modeling of Planar Defects in Solid Solutions by the Special Quasirandom Structure Approach."

148. University of California, Davis, MRS Student Chapter Seminar, May 24, 2013, "Using Computation to Aid Materials Discovery and Design."

149. Fundamentals of Thermodynamic Modelling of Materials Summer School, INSTN – CEA, Saclay, France, July 5, 2013, "Modelling Liquids from First Principles."

150. TMS Integrated Computational Materials Engineering Congress, Salt Lake City, UT, July 11, 2013, "Integrated Computational Materials Education."

151. Department of Energy Materials Genome Initiative PI Meeting, Washington, DC, July 19, 2013, "The Materials Project – A Public Design Platform."

152. Glenn T. Seaborg Center Seminar, Lawrence Berkeley National Laboratory, Berkeley, CA, October 2, 2013, "First-Principles Modeling of the Thermochemistry of Actinide Oxide Solid Solutions."

153. Phase Stability, Diffusion, Kinetics and Their Applications (PSDK-VIII) Symposium, Session Honoring Peter Voorhees, Recipient of ASM's 2013 J. Willard Gibbs Phase Equilibria Award, MS&T13 Conference, Montreal, Canada, October 28, 2013, "Growth Processes at Faceted Solid-Liquid Interfaces Studied by Molecular Dynamics Simulations."

154. Phase Stability, Diffusion, Kinetics and Their Applications (PSDK-VIII) Symposium, MS&T13 Conference, Montreal, Canada, October 28, 2013, "First-Principles Calculations of Diffusion Coefficients in Support of the Design of Ferritic Superalloys."

155. Thermec 2013 – International Conference on Processing & Manufacturing of Advanced Materials, Las Vegas, NV, December 2, 2013, "Structural Phase Transitions in Metallic Grain Boundaries." *Keynote lecture*.

156. Computational Thermodynamics and Kinetics Symposium, TMS Annual Meeting, San Diego, CA, February 17, 2014, "Atomistic Simulation Studies of Materials Interfaces: Recent Insights and Remaining Challenges."

157. Invited Session: Materials Genome: Theory-Led Accelerated Materials Discovery, American Physical Society March Meeting, Denver, CO, March 3, 2014, "Materials Data for Accelerated Discovery and Design."

158. Georgia Institute of Technology, Materials Science and Engineering Colloquium, March 24, 2014, "Behavior at the Edge – Insights into the Properties of Materials Interfaces from Computer Simulations."

159. American Association for Crystal Growth and Epitaxy (AACGE) Western Sectional Meeting, Stanford Sierra Camp, Fallen Leaf Lake, CA, June 10, 2014, "Insights into Faceted Crystal Growth in Bulk and Nanowire Geometries from Molecular Dynamics Simulations."

160. School for Advanced Thermodynamic Assessments, Centre Port-Royal, France, June 24, 2014, "First-Principles Methods for Alloy Thermodynamic Properties."

161. City University of Hong Kong, 30th Anniversary Technology Forum, Hong Kong, September 22, 2014, "Materials Discovery and Design: The Enabling Role of Computational Modeling."

162. City University of Hong Kong, Department of Physics and Materials Science Seminar, Hong Kong, September 24, 2014, "Behavior at the Edge – Insights into the Properties of Materials Interfaces from Computer Simulations."

163. 7th International Conference on Multiscale Materials Modeling, Berkeley, CA, October 8, 2014, "Role of Multiscale Materials Modeling in Integrated Computational Materials Engineering." (Plenary Lecture)

164. Symposium on Interfaces, Grain Boundaries and Surfaces from Atomistic and Macroscopic Approaches: Fundamental and Engineering Issues, MS&T 2014, Pittsburgh, PA, October 14, 2014, "Wetting Instability in Nanowire Geometries." (Keynote Lecture)

165. University of Minnesota, Department of Chemical Engineering and Materials Science Colloquium, December 9, 2014, "Behavior at the Edge – Insights into the Properties of Materials Interfaces from Computer Simulations."

166. Computational Modeling and Stochastic Methods for Materials Discovery and Properties Symposium, TMS Annual Meeting, Orlando, FL, March 16, 2015, "Computational Database for Elastic Properties of Materials."

167. 2015 DPG Spring Meeting (Deutschen Physikalischen Gesellschaft – Frühjahrstagung), Berlin, Germany, March 18, 2015, "Computationally Aided Materials Discovery and Design." (Plenary Lecture)

168. University of Pennsylvania, Department of Materials Science and Engineering Colloquium, March 26, 2015, "Behavior at the Edge – Insights into the Properties of Materials Interfaces from Computer Simulations."

169. Duke University, Department of Mechanical Engineering and Materials Science Persall Distinguished Lecture, April 13, 2015, "Computational Aided Materials Discovery and Design."

170. University of California, Santa Barbara, Materials Department Colloquium, May 22, 2015, "New Insights into Mechanical Deformation in Metals from Synergistic Experimental and Computational Studies."

171. The Future of Graduate Education in Materials Workshop, University of California, Santa Barbara, June 11, 2015, "Needs for the Graduate Curriculum: Theory and Computation."

172. Atomistic Simulations of Interfaces Symposium, Solid-Solid Phase Transformations in Inorganic Materials (PTM 2015) Meeting, Whistler, British Columbia, Canada, June 29, 2015, "Structural Phase Transitions in Solid-Solid Interfaces and Their Effect on Kinetic Properties."

173. School for Advanced Thermodynamic Assessments, Centre Port-Royal, France, July 7, 2015, "First-Principles Methods: An Introduction."

174. SanDisk Corporation, Milpitas, CA, July 22, 2015, "Computationally Aided Materials Discovery and Design."

175. University of Illinois, Urbana-Champaign, Materials Science and Engineering Department Colloquium, September 21, 2015, "Computational Modeling for Materials Discovery and Design."

176. Materials Research Society, Boston, MA, November 30, 2015, "Energetics of Twinning in HCP Transition Metals."

177. North Carolina State University, Materials Science and Engineering Department Colloquium, December 4, 2015, "Computational Modeling for Materials Discovery and Design."

178. Frontiers in Solidification: An MPMD Symposium in Honor of Michel Rappaz, TMS Annual Meeting, Nashville, TN, February 15, 2016, "Charting the Elastic Properties of Crystalline Inorganic Compounds."

179. Hume-Rothery Award Symposium: Thermodynamics of Materials, TMS Annual Meeting, Nashville, TN, February 15, 2016, "Charting the Elastic Properties of Crystalline Inorganic Compounds."

180. Morris E. Fine Lecture, Department of Materials Science and Engineering, Northwestern University, Evanston, IL, March 1, 2016, "Twinning in HCP Metals: Anomalous Energetics and How They May Be Useful."

181. Symposium on Recent Developments in Mathematical Modeling of Recrystallization, Grain Growth and Related Phenomena, SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia, PA, May 8, 2016, "Atomistic Simulations of Line Defects at Interfaces."

182. Intermolecular, Inc., San Jose, CA, June 3, 2016, "Computational Modeling for Materials Discovery and Design."

183. Symposium on Modelling and Simulation of Microstructures and Processing, 9th Pacific Rim International Conference on Advanced Materials and Processing (PRICM9), Kyoto, Japan, August 4, 2016, "Atomistic Simulations of Line Defects at Interfaces."

184. Materials Science and Engineering Distinguished Seminar Series, University of Central Florida, Orlando, FL, September 26, 2016, "Computational Modeling for Materials Discovery."

185. 8th International Conference on Multiscale Modeling of Materials, Dijon, France, October 10, 2016, "Multiscale Modeling of Coherent Precipitation in Interstitial Solid Solutions."

186. NuMat (The Nuclear Materials Conference) 2016, Montpellier, France, November 8, 2016, "Energetics of Trivalent Substitutional Elements in Actinide Dioxides: Combined Computational and Experimental Investigations."

187. Materials Research Society, Boston, MA, November 29, 2016, "Computer Simulation Study of Effects of Pressure on Structure, Stability and Properties of Metallic Glasses."

188. The John Cahn Memorial Symposium, TMS Annual Meeting, San Diego, CA, March 1, 2017, "Energetics Trends for Twin Boundaries in HCP Metals."

189. Computational Thermodynamics and Kinetics Symposium, TMS Annual Meeting, San Diego, CA, March 1, 2017, "First-Principles Calculations of Coherent Phase Equilibria and Short-Range-Order Hardening in the α-Ti-O System."

190. Microstructural Processes in Irradiated Materials Symposium, TMS Annual Meeting, San Diego, CA, March 2, 2017, "Energetics of Trivalent Substitutional Elements in Uranium Dioxide: Combined Computational and Experimental Investigations."

191. Materials Science and Engineering Colloquium, Arizona State University, Tempe, AZ, March 31, 2017, "Computational Modeling for Materials Discovery."

192. Emergent Material Properties and Phase Transitions Under Pressure Symposium, MRS Spring Meeting, Phoenix, AZ, April 18, 2017, "A Statistical Learning Model for Elastic Moduli of Inorganic Compounds: Application to Discovery of New Superhard Materials."

193. Materials Science and Engineering Colloquium, Stanford University, Stanford, CA, May 26, 2017, "Computational Modeling in the Discovery and Design of Structural Materials."

194. ET Guest Lecture Series Seminar, Applied Materials, Santa Clara, CA, May 30, 2017, "Computational Modeling for Materials Discovery and Design."

195. 100 Year Anniversary Colloquium, Max Planck Institut fur Eisenforschung, Duesseldorf, Germany, October 5, 2017, "Computational Materials Science: An Enabling Framework for Accelerated Materials Discovery and Design."

196. Hume-Rothery Award Symposium, TMS Annual Meeting, Phoenix, AZ, March 12, 2018, "Automating First-Principles Calculations of Point Defect Thermodynamics."

197. Non-Equilibrium Features of Grain Boundaries Symposium, TMS Annual Meeting, Phoenix, AZ, March 13, 2018, "Dislocations, Twins, Grain Boundaries and Their Interactions in HCP Rhenium."

198. 10-Years ICAMS International Symposium, Ruhr University Bochum, Bochum, Germany, June 27, 2018, "Insights into Deformation Mechanisms from Atomistic Simulations – The Case of Oxygen in Titanium."

199. Hume-Rothery Award Symposium, TMS Annual Meeting, San Antonio, TX, March 11, 2019, "Order Within Disordered Materials: Insights into the Nature and Impact of Short-Range-Order in Concentrated Solid Solutions."

200. Materials Science and Engineering Division Colloquium, National Institute of Standards and Technology, Gaithersburg, MD, July 13, 2018, "Accelerated Design of Structural Materials: A Case Study Involving Replacement Alloys for Rhenium."

201. National Academies' Materials and Manufacturing Board Focus Session on High Entropy Alloys, Panel Member, Washington, DC, October 10, 2018.

202. ICME Education in Materials Science and Mechanical Engineering Symposium, TMS Annual Meeting, San Antonio, TX, March 14, 2019, "Computational Materials Science & Engineering Education: Present & Future."

203. Symposium on New Frontiers in the Confluence of Experimental Thermodynamics, Structural Investigations and Theory/Computation, ACS National Meeting, Orlando, FL, April 1, 2019, "Epitaxial Stabilization of Polar Phases in ABO_3 Compounds: High-Throughput Computational Study."

204. Plenary talk on Nuclear Materials, National Laboratory Chief Research Officer (NLCRO) Materials Science Working Group Workshop on Materials Synthesis, April 9, 2019.

205. Symposium on Interfacial Science and Engineering – Mechanics, Thermodynamics, Kinetics and Chemistry, MRS Spring Meeting, Phoenix, AZ, April 26, 2019, "Twinning in Multi-Principal-Element Alloys – Atomistic Simulation Studies."

206. Phase Stability and Diffusion Kinetics XIV Symposium, MS&T Meeting, Portland, OR, September 30, 2019, "Short-Range Order Effects Related to Mechanical Properties in Concentrated Solid Solutions."

207. Young Professional Luncheon Tutorial Lecture, MS&T Meeting, Portland, OR, October 1, 2019, "Perspectives from a Career Trajectory through the National Labs to Academia (and Back Again)."

208. Hume-Rothery Award Symposium, TMS Annual Meeting, San Diego, CA, February 24, 2020, "Hexagonal Close Packed Multi-Principal-Element Alloys Identified Computationally."

209. High-Entropy and Compositionally Complex Alloys Symposium, 2020 MRS Virtual Spring/Fall Meeting, November 27 – December 4, 2020, "Atomic Scale Computational Investigations of Dislocation in BCC High Entropy Alloys."

210. Processing Structure–Property Relationship of Advanced Intermetallic-Based Alloys for Structural and Functional Applications Symposium, 2020 MRS Virtual Spring/Fall Meeting, November 27 – December 4, 2020, "A Hexagonal Close Packed Multi-Principal-Element Alloy Identified Computationally" (Presented in live keynote session on December 3, 2020).

211. Materials Research Lecture, California Institute of Technology, "Computationally Guided Alloy Design through Control of Bulk and Interfacial Phases," March 3, 2021.

212. Materials Science Seminar, University of Cincinnati, "Computationally Guided Alloy Design through Control of Bulk and Interfacial Phases," April 16, 2021.

213. Materials Science Seminar, Oregon State University, "Computationally Guided Alloy Design through Control of Bulk and Interfacial Phases," May 27, 2021.

214. CAMD/MURI/AFLOW Seminar, Duke University, "Computationally Guided Alloy Design through Control of Bulk and Interfacial Phases," July 8, 2021.

215. PSDK XV Symposium: Gibbs Award Session, 2021 IMAT (International Materials, Applications & Technologies) Annual Meeting, "The Connection Between Bulk and Interfacial Phases in a Titanium Twin Boundary," September 14, 2021.

216. Hume-Rothery Award Symposium, TMS Annual Meeting, Anaheim, CA, February 28, 2022, "Molecular-Scale Structure & Dynamics of Molten Salts: Simulations and Implications for Corrosive Processes."

217. Grain Boundaries and Interfaces Symposium, TMS Annual Meeting, Anaheim, CA, March 2, 2022, "Twin-Boundary Structural Phase Transition in HCP Titanium."

218. The National Academies Defense Materials Manufacturing and its Infrastructure (DMMI) Workshop on High Temperature Materials Systems: Emerging Applications, Materials and Science Gaps, Washington, DC, May 11, 2022, "Computational Approaches to High Temperature Systems: A Case Study in Alloy Design of Rhenium Alternatives."

219. International Research Conference on Structure and Thermodynamics of Oxides/Carbides/Nitrides/Borides at High Temperatures, October 6, 2022, "Associates, Solvation and Speciation in Molten Salts: Insights from Molecular Dynamics Simulations."

220. Local Ordering in Materials and Its Impacts on Mechanical Behaviors, Radiation Damage, and Corrosion Symposium, TMS Annual Meeting, San Diego, CA, March 21, 2023, "Short-Range Order Effects on Dislocation Mobilities in High-Entropy Alloys from Atomistic Simulations."

221. Alloy Behavior and Design Across Length-Scales Symposium, TMS Annual Meeting, San Diego, CA, March 21, 2023, "Deformation Twinning in HCP-Ti – Role of Interfacial Complexions and Interstitial Solutes."

222. Frontiers in Solidification Symposium, TMS Annual Meeting, San Diego, CA, March 21, 2023, "Dealloying of Metals in Molten Salts – From Atomistic to Mesoscale Simulations."

223. Advanced Engineering Materials Workshop, Lawrence Livermore National Laboratory, Livermore, CA, March 28, 2023, "Short-Range Order Effects on Dislocation Mobilities in High-Entropy Alloys from Atomistic Simulations."

224. International Conference on High-Entropy Materials, Knoxville, TN, June 21, 2023, "Local Lattice Distortions and Structural Instabilities in Nb-Ta-Ti-Hf High-Entropy Alloys."

225. The Seidman Family Lecture Series, Tel-Aviv University, Tel-Aviv, Israel, July 12, 2023, "Local Order In High-Entropy Alloys."

226. The Seidman Family Lecture Series, Tel-Aviv University, Tel-Aviv, Israel, July 13, 2023, "Interfacial Complexions and Metastable Polymorphs."

227. Materials Research Society, Boston, MA, November 28, 2023, "Concentrated Alloys: Order, Disorder and the Vast Space in Between."