Dallas R. Trinkle

2018 March 29

Curriculum Vitæ

University of Illinois, Urbana-Champaign
Materials Science and Engineering
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Professional Preparation

Xavier University	B.S., Physics and Mathematics	1996
Ohio State University	Ph.D., Physics	2003
	Advisors: Prof. John W. Wilkins and Dr. Robert C. Albers	
Air Force Research Laboratory	Postdoc, Materials and Manufacturing Directorate	2004–06
	Advisor: Dr. Christopher Woodward	

Appointments

2012–	Associate Professor, Materials Science and Engineering, Materials Research Laboratory, and Computational Science and Engineering, UIUC
9–12/2017	Senior Research Fellow, Institute for Pure and Applied Mathematics, UCLA
9–12/2012	Senior Research Fellow, Institute for Pure and Applied Mathematics, UCLA
2006–2012	Assistant Professor, Materials Science and Engineering, UIUC
2011–2012	Assistant Professor, Materials Research Laboratory, UIUC
2009–2012	Affiliated Assistant Professor, Nuclear, Plasma, and Radiological Eng., UIUC
2005–2008	Adjunct Assistant Professor of Physics, Ohio State University
2004–2006	National Research Council Postdoctoral Associate, Air Force Research Laboratory
2001–2003	Graduate Research Assistant, Ohio State University
2000–2001	Fowler Fellow, Ohio State University
1998–2000	Graduate Research Assistant, Los Alamos National Laboratory, Group T-11
1996–1998	Fowler Fellow, Ohio State University

Academic Honors

NCSA Faculty Fellow (2017)	*Univ. Illinois*
Center for Advanced Study Associate (2017)	*Univ. Illinois*
Willett Faculty Scholar Award (2015)	*Univ. Illinois*
AIME Robert Lansing Hardy Award (2014)	*TMS-AIME*
Xerox Faculty Research Award (2011)	*Univ. Illinois*
Early Career Fellow, Honorable Mention (2011)	*TMS*
Faculty Early Career Development Award (CAREER, 2009)	*NSF/CMMI*
3M Untenured Faculty Research Award (2008, 2009, 2010)	*3M*
Young Leader International Scholar Award (2008)	*TMS*
Young Leader Intern (Professional Development Award) Structural Materials Division (2006)	*TMS*
National Research Council Associate (2004–2006)	*Air Force Research Laboratory*
Fowler Fellow (1996–1998, 2000–2001)	*Ohio State University*

Professional Activities

Editorial Review Board for *Integrating Materials and Manufacturing Innovation*, 2012–
Co-chair, 2011 Physical Metallurgy Gordon conference
TMS technical committees: Computational Materials Science and Engineering (vice-chair 2012–2014; chair 2014–2016); Chemistry and Physics of Materials (vice-chair 2015–2018; chair 2018–); Magnesium; Integrated Computational Materials Engineering

TMS service committees: Nominating Committee (2012–2016), Young Leaders (2006–2012)
Organizer, 2017 TMS annual meeting "Computational Materials Discovery and Optimization: From 2D to Bulk Materials" symposium
Organizer, 2016 TMS annual meeting "Computational Methods for Spatio-temporal Scale-bridging: from Atomistics to Mesoscale" symposium
Organizer, 2016 TMS annual meeting "Computational Materials Discovery and Optimization: From 2D to Bulk Materials" symposium
Organizer, 2015 TMS annual meeting "Computational Discovery of Novel Materials" symposium
Organizer, 2014 TMS annual meeting "Computational Discovery of Novel Materials" symposium
Organizer, 2014 TMS annual meeting "Computational Thermodynamics and Kinetics" symposium
Organizer, 2014 TMS annual meeting "Multiscale Perspectives on Plasticity in HCP Metals" symposium
Organizer, 2013 TMS annual meeting "Computational Discovery of Novel Materials" symposium
Organizer, 2012 TMS annual meeting "Stochastic Methods in Materials Research" symposium
Organizer, 2012 TMS annual meeting "Minerals, Metals & Materials under Pressure" symposium
Organizer, 2010 TMS annual meeting "Stochastic Methods in Materials Research" symposium
Organizer, 2010 TMS annual meeting "Computational Thermodynamics and Kinetics" symposium
Organizer, 2008 TMS annual meeting "Minerals, Metals & Materials under Pressure" symposium
Organizer, 2006 TMS annual meeting "Point Defects in Materials" symposium
Organizer, 2008 "Recent Developments in Electronic Structure Methods" workshop, UIUC
Organizer, 2006 "Recent Developments in Electronic Structure Methods" workshop, OSU
NSF TeraGrid Allocations Committee Reviewer (2008–2011)
Proposal reviews: DOE: BES, NSF: MPS, NSF: ENG
Manuscript reviews: Phys. Rev. Lett., Phys. Rev. B, J. Phys. Chem., J. Phys: CM, Acta Mat., Phil. Mag., J. Math. Phys., Comp. Mat. Sci., Model. Sim. Mater. Sci. Eng.
Organizer, 2007–2014 ASM Materials Camp for high school teachers, UIUC
Organizer, 2011–2014 Girls Learning About Materials (GLAM) summer camp for high school seniors, UIUC
2014–2017 Education Innovation Fellow, College of Engineering, UIUC

Current Research Grants

6. *USAMP Low-Cost Mg Sheet Component Development and Demonstration Project.* USAMP; DOE/EERE.
5. *PIRE: Integrated Computational Materials Engineering for Active Materials and Interfaces in Chemical Fuel Production.* N. R. Aluru; NSF.
4. *DMREF/GOALI/Collaborative Research: Computational Design, Rapid Processing and Characterization of Multiple Classes of Materials to Accelerate Materials Innovation.* K. S. Ravi Chandran (Univ. Utah), D. R. Trinkle, and A. P. Sanders (Ortho Development); NSF/CMMI.
3. *Surface and Interface Free Energies of Epitaxial Nanocrystals.* J. Zuo and D. R. Trinkle; NSF/DMR.
2. *Materials for Extreme Irradiation Environments.* Illinois MRL Cluster; DOE/BES.
1. *Engineered Zircaloy Cladding and Fuel Pellet Modifications for Improved Accident Tolerance of LWR Nuclear Fuel.* Multi-institutional grant; DOE/NEUP.

Past Research Grants

12. *GOALI: Experimentally-Validated Computational Approach to Developing and Predicting Kinetics in Anisotropic Systems.* D. R. Trinkle, M. Manuel (Univ. Florida), C. Jiang (Thermo-Calc), and K. Wu (ThermoCalc); NSF/CDSE (09/01/2014–08/31/2017).
11. *High-throughput discovery of thermally-functional materials.* D. Cahill, D. Shoemaker, D. R. Trinkle; Toyota (3/1/16–2/28/17).
10. *Integrated Computational Approach to Development of Lightweight 3GAHSS Vehicle Sub-Assembly.* Multi-institutional grant, USAMP/ASP; DOE/EERE (10/01/12–09/30/16).
9. *Enhanced Diffusivity Along Dislocations from Quantum Tunneling to Classical Transport in the PD-H System.* B. Heuser and D. R. Trinkle; NSF/DMR (08/15/12–07/31/15).
8. *First Principles Calculation of Oxygen and Oxygen-Solute Effects on Deformation in Titanium.* D. R. Trinkle; ONR (07/01/12–06/30/15).
7. *The Role of Point Defects in the Structure and Properties of Perovskites for Functional Applications.* R. Ubic (Boise State), W. Kriven, D. R. Trinkle; NSF (10/01/2010–09/30/2014).
6. *Surface and Interface Free Energies of Epitaxial Nanocrystals.* J. Zuo and D. R. Trinkle; NSF/DMR (07/01/10–06/30/14).
5. *CAREER: First-Principles Modeling of Titanium-Oxygen-Solute Interaction: Materials Design for Improved Energy Efficiency.* D. R. Trinkle; NSF/CMMI (01/15/09–01/14/14).
4. *Hydrogen-dislocation interactions at low temperature in deformed Pd: Spatial and vibrational characterization using neutron scattering and advanced computational techniques.* B. Heuser and D. R. Trinkle; NSF/DMR (06/15/08–08/14/12).
3. *GOALI: Modeling solute effects in magnesium alloys: First-principles to predictive finite-element.* D. R. Trinkle and L. G. Hector, Jr. (General Motors); NSF/CMMI (08/01/08–07/31/12).
2. *Designing Oxygen-tolerant Titanium Alloys with First-principles.* D. R. Trinkle; Boeing (06/15/09–06/15/11).
1. *Heteroepitaxial metal nanostructure diffusion through collective slip.* J. Weaver and D. R. Trinkle; NSF/DMR (06/15/07–06/14/10).

Refereed Publications

67. *Ab initio magnesium-solute transport database using exact diffusion theory.*
R. Agarwal and D. R. Trinkle.
Acta mater. **150**, 339–350 (2018), doi://10.1016/j.actamat.2018.03.025.
Database: dx.doi.org/10.18126/M20G83
66. *Solute-induced solid-solution softening and hardening in bcc tungsten.*
Y.-J. Hu, M. R. Fellinger, B. G. Bulter, Y. Wang, K. A. Darling, L. J. Kecskes, D. R. Trinkle, and Z.-K. Liu.
Acta mater. **141**, 304–316 (2017), doi://10.1016/j.actamat.2017.09.019
65. *Automatic numerical evaluation of vacancy-mediated transport for arbitrary crystals: Onsager coefficients in the dilute limit using a Green function approach.*
D. R. Trinkle.
Philos. Mag. **97**, 2514–2563 (2017), doi://10.1080/14786435.2017.1340685
64. *Mechanical properties and phase stability of monoborides using density functional theory calculations.*
H. Kim and D. R. Trinkle.
Phys. Rev. Mater. **1**, 013601 (2017), doi://10.1103/PhysRevMaterials.1.013601.
Database: dx.doi.org/10.18126/M24S3J

63. *Design principles for radiation-resistant solid solutions.*
T. Schuler, D. R. Trinkle, P. Bellon, and R. Averback.
Phys. Rev. B **95**, 174102 (2017), doi://10.1103/PhysRevB.95.174102
62. *Mesoscale modeling of vacancy-mediated Si segregation near an edge dislocation in Ni under irradiation.*
Z. Li and D. R. Trinkle.
Phys. Rev. B **95**, 144107 (2017), doi://10.1103/PhysRevB.95.144107
61. *Exact model of vacancy-mediated solute transport in magnesium.*
R. Agarwal and D. R. Trinkle.
Phys. Rev. Lett. **118**, 105901 (2017), doi://10.1103/PhysRevLett.118.105901
60. *Ab initio calculations of the lattice parameter and elastic stiffness coefficients of bcc Fe with solutes.*
M. R. Fellinger, L. G. Hector, Jr., and D. R. Trinkle.
Comp. Mater. Sci. **126**, 503–513 (2017), doi://10.1016/j.commatsci.2016.09.040.
Database: hdl.handle.net/11256/671
59. *First principles calculations of beryllium stability in zirconium surfaces.*
A. C. P. Jain and D. R. Trinkle.
Acta mater. **122**, 359–368 (2017), doi://10.1016/j.actamat.2016.10.003
58. *Reforming an undergraduate materials science curriculum with computational modules.*
R. Mansbach, A. Ferguson, K. Kilian, J. Krogstad, C. Leal, A. Schleife, D. R. Trinkle, M. West, and G. L. Herman.
J. Mater. Edu. **38**, 161–174 (2016)
57. *Ab initio modeling of quasielastic neutron scattering of hydrogen pipe diffusion in palladium.*
E. J. Schiavone and D. R. Trinkle.
Phys. Rev. B **94**, 054114 (2016), doi://10.1103/PhysRevB.94.054114
56. *Light element diffusion in Mg using first principles calculations: Anisotropy and elastodiffusion.*
R. Agarwal and D. R. Trinkle.
Phys. Rev. B **94**, 054106 (2016), doi://10.1103/PhysRevB.94.054106.
Database: hdl.handle.net/11256/694
55. *Computation of the lattice Green function for a dislocation.*
A. M. Z. Tan and D. R. Trinkle.
Phys. Rev. E **94**, 023308 (2016), doi://10.1103/PhysRevE.94.023308
54. *A modified embedded atom method potential for interstitial oxygen in titanium.*
P. Zhang and D. R. Trinkle.
Comp. Mater. Sci. **124**, 204–210 (2016), doi://10.1016/j.commatsci.2016.07.039.
Database: hdl.handle.net/11256/782
53. *Diffusivity and derivatives for interstitial solutes: Activation energy, volume, and elastodiffusion tensors.*
D. R. Trinkle.
Philos. Mag. **96**, 2714–2735 (2016), doi://10.1080/14786435.2016.1212175
52. *Oxygen diffusion in HCP metals.*
H. H. Wu, P. Wisesa, and D. R. Trinkle.
Phys. Rev. B **94**, 014307 (2016), doi://10.1103/PhysRevB.94.014307
51. *Kinetic monte carlo investigation of tetragonal strain on Onsager matrices.*
Z. Li and D. R. Trinkle.
Phys. Rev. E **93**, 053305 (2016), doi://10.1103/PhysRevE.93.053305

50. *Size misfits of point defects in aliovalently doped $SrTiO_3$ using density functional theory*.
H. Kim and D. R. Trinkle.
Comp. Mater. Sci. **119**, 41–45 (2016), doi://10.1016/j.commatsci.2016.02.040
49. *A study of stress relaxation in AZ31 using high-energy X-ray diffraction*.
W. Tang, K. L. Halm, D. R. Trinkle, M. Koker, U. Lienert, P. Kenesei, and A. J. Beaudoin.
Acta mater. **101**, 71–79 (2015), doi://10.1016/j.actamat.2015.08.072
48. *Energetics of rutile TiO_2 vicinal surfaces with $\langle 001 \rangle$ steps from the energy density method*.
B. Lee and D. R. Trinkle.
J. Phys. Chem. C **119**, 18203–18209 (2015), doi://10.1021/acs.jpcc.5b03623
47. *Database optimization for empirical interatomic potential models*.
P. Zhang and D. R. Trinkle.
Model. Simul. Mater. Sci. Eng. **23**, 065011 (2015), doi://10.1088/0965-0393/23/6/065011
46. *Importance of coordination number and bond length in titanium revealed by electronic structure investigations*.
L.-F. Huang, B. Grabowski, E. McEniry, D. R. Trinkle, and J. Neugebauer.
Phys. Stat. Solid. B **252**, 1907–1924 (2015), doi://10.1002/pssb.201552280
45. *Thermal transport across high-pressure semiconductor-metal transition in Si and $Si_{0.991}Ge_{0.009}$*.
G. T. Hohensee, M. R. Fellinger, D. R. Trinkle, and D. G. Cahill.
Phys. Rev. B **91**, 205104 (2015), doi://10.1103/PhysRevB.91.205104
44. *Calculation of strain effects on vacancy-mediated diffusion of impurities in FCC structures: General approach and application to $Ni_{1-x}Si$*.
T. Garnier, Z. Li, M. Nastar, P. Bellon, and D. R. Trinkle.
Phys. Rev. B **90**, 184301 (2014), doi://10.1103/PhysRevB.90.184301
43. *Diffusion of Si impurities in Ni under stress: A first-principles study*.
T. Garnier, V. R. Manga, P. Bellon, and D. R. Trinkle.
Phys. Rev. B **90**, 024306 (2014), doi://10.1103/PhysRevB.90.024306.
Database: hdl.handle.net/11115/239
42. *Direct measurement of hydrogen dislocation pipe diffusion in deformed polycrystalline Pd using quasielastic neutron scattering*.
B. J. Heuser, D. R. Trinkle, N. Jalarvo, J. Serio, E. J. Schiavone, E. Mamontov, and M. Tyagi.
Phys. Rev. Lett. **113**, 025504 (2014), doi://10.1103/PhysRevLett.113.025504
41. *Interaction of oxygen interstitials with lattice faults in Ti*.
M. Ghazisaeidi and D. R. Trinkle.
Acta mater. **76**, 82–86 (2014), doi://10.1016/j.actamat.2014.05.025
40. *First-principles study of interfacial boundaries in Ni–Ni_3Al*.
C. Woodward, A. van de Walle, M. Asta, and D. R. Trinkle.
Acta mater. **75**, 60–70 (2014), doi://10.1016/j.actamat.2014.04.056
39. *Quantitative modeling of solute drag by vacancies in face-centered-cubic alloys*.
T. Garnier, D. R. Trinkle, M. Nastar, and P. Bellon.
Phys. Rev. B **89**, 144202 (2014), doi://10.1103/PhysRevB.89.144202
38. *Stress-induced anisotropic diffusion in alloys: Complex Si solute flow near a dislocation core in Ni*.
T. Garnier, V. R. Manga, D. R. Trinkle, M. Nastar, and P. Bellon.
Phys. Rev. B **88**, 134108 (2013), doi://10.1103/PhysRevB.88.134108
37. *Solute drag by vacancies in body-centered cubic alloys*.
T. Garnier, M. Nastar, P. Bellon, and D. R. Trinkle.
Phys. Rev. B **88**, 134201 (2013), doi://10.1103/PhysRevB.88.134201

36. *Solute effect on oxygen diffusion in α-titanium.*
H. H. Wu and D. R. Trinkle.
J. Appl. Phys. **113**, 223504 (2013), doi://10.1063/1.4808283.
Database: hdl.handle.net/11115/125
35. *Hydrogen trapping at dislocation cores at room temperature in deformed Pd.*
B. J. Heuser, D. R. Trinkle, T.-N. Yang, and L. He.
J. Alloy. Compd. **577**, 189–191 (2013), doi://10.1016/j.jallcom.2013.04.082
34. *Ab initio based empirical potential used to study the mechanical properties of molybdenum.*
H. Park, M. R. Fellinger, T. J. Lenosky, W. W. Tipton, D. R. Trinkle, S. P. Rudin, C. Woodward, J. W. Wilkins, and R. G. Hennig.
Phys. Rev. B **85**, 214121 (2012), doi://10.1103/PhysRevB.85.214121
33. *Direct calculation of lattice green function with arbitrary interactions for general crystals.*
J. A. Yasi and D. R. Trinkle.
Phys. Rev. E **85**, 066706 (2012), doi://10.1103/PhysRevE.85.066706
32. *Prediction of thermal cross-slip stress in magnesium alloys from a geometric interaction model.*
J. A. Yasi, L. G. Hector, Jr., and D. R. Trinkle.
Acta mater. **60**, 2350–2358 (2012), doi://10.1016/j.actamat.2012.01.004
31. *Core structure of a screw dislocation in Ti from density functional theory and classical potentials.*
M. Ghazisaeidi and D. R. Trinkle.
Acta mater. **60**, 1287–1292 (2012), doi://10.1016/j.actamat.2011.11.024
30. *Au/TiO_2(110) interfacial reconstruction stability from ab initio.*
M. Yu and D. R. Trinkle.
J. Phys. Chem. C **115**, 17799–17805 (2011), doi://10.1021/jp2017133
29. *Direct diffusion through interpenetrating networks: Oxygen in titanium.*
H. H. Wu and D. R. Trinkle.
Phys. Rev. Lett. **107**, 045504 (2011), doi://10.1103/PhysRevLett.107.045504
28. *Prediction of thermal cross-slip stress in magnesium alloys from direct first principles data.*
J. A. Yasi, L. G. Hector, Jr., and D. R. Trinkle.
Acta mater. **59**, 5652–5660 (2011), doi://10.1016/j.actamat.2011.05.040
27. *Nanoscale-hydride formation at dislocations in palladium: Ab initio theory and inelastic neutron scattering measurements.*
D. R. Trinkle, H. Ju, B. J. Heuser, and T. J. Udovic.
Phys. Rev. B **83**, 174116 (2011), doi://10.1103/PhysRevB.83.174116
26. *Thermal conductivity of compressed H_2O to 22 GPa: A test of the Leibfried-Schlömann equation.*
B. Chen, W.-P. Hsieh, D. G. Cahill, D. R. Trinkle, and J. Li.
Phys. Rev. B **83**, 132301 (2011), doi://10.1103/PhysRevB.83.132301
25. *Energy density in density functional theory: Application to crystalline defects and surfaces.*
M. Yu, D. R. Trinkle, and R. M. Martin.
Phys. Rev. B **83**, 115113 (2011), doi://10.1103/PhysRevB.83.115113
24. *Accurate and efficient algorithm for Bader charge integration.*
M. Yu and D. R. Trinkle.
J. Chem. Phys. **134**, 064111 (2011), doi://10.1063/1.3553716

23. *First-principles calculation of H vibrational excitations at a dislocation core of Pd*.
H. M. Lawler and D. R. Trinkle.
Phys. Rev. B **82**, 172101 (2010), doi://10.1103/PhysRevB.82.172101
22. *Misfit-dislocation-mediated island diffusion: Cu on Ag(111)*.
A. W. Signor, H. H. Wu, and D. R. Trinkle.
Surf. Sci. Lett. **604**, 67–70 (2010), doi://10.1016/j.susc.2010.08.003
21. *Lattice green's function for crystals containing a planar interface*.
M. Ghazisaeidi and D. R. Trinkle.
Phys. Rev. B **82**, 064115 (2010), doi://10.1103/PhysRevB.82.064115
20. *First-principles data for solid-solution strengthening of magnesium: From geometry and chemistry to properties*.
J. A. Yasi, L. G. Hector, Jr., and D. R. Trinkle.
Acta mater. **58**, 5704–5713 (2010), doi://10.1016/j.actamat.2010.06.045
19. *Island shape controls magic-size effect for heteroepitaxial diffusion*.
H. H. Wu, A. W. Signor, and D. R. Trinkle.
J. Appl. Phys. **108**, 023521 (2010), doi://10.1063/1.3455848
18. *Ab initio simulations of molten Ni alloys*.
C. Woodward, M. Asta, D. R. Trinkle, J. Lill, and S. Angioletti-Uberti.
J. Appl. Phys. **107**, 113522 (2010), doi://10.1063/1.3437644
17. *Atomistic study of edge and screw $\langle c + a \rangle$ dislocations in magnesium*.
T. Nogaret, W. A. Curtin, J. A. Yasi, L. G. Hector, Jr., and D. R. Trinkle.
Acta mater. **58**, 4332–4343 (2010), doi://10.1016/j.actamat.2010.04.022
16. *Cu/Ag EAM potential optimized for heteroepitaxial diffusion from ab initio data*.
H. H. Wu and D. R. Trinkle.
Comp. Mater. Sci. **47**, 577–583 (2009), doi://10.1016/j.commatsci.2009.09.026
15. *Basal and prism dislocation cores in magnesium: Comparison of first-principles and embedded-atom-potential methods predictions*.
J. A. Yasi, T. Nogaret, D. R. Trinkle, Y. Qi, L. G. Hector, Jr., and W. A. Curtin.
Model. Simul. Mater. Sci. Eng. **17**, 055012 (2009), doi://10.1088/0965-0393/17/5/055012
14. *Convergence rate for numerical computation of the lattice Green's function*.
M. Ghazisaeidi and D. R. Trinkle.
Phys. Rev. E **79**, 037701 (2009), doi://10.1103/PhysRevE.79.037701
13. *Mechanism of a prototypical synthetic membrane-active antimicrobial: Efficient hole-punching via interaction with negative intrinsic curvature lipids*.
L. Yang, V. D. Gordon, D. R. Trinkle, N. W. Schmidt, M. A. Davis, C. DeVries, A. Som, J. E. Cronan, Jr., G. N. Tew, and G. C. L. Wong.
Proc. Nat. Acad. Sci. **105**, 20595 (2008), doi://10.1073/pnas.0806456105
12. *Classical potential describes martensitic phase transformations between the α, β and ω titanium phases*.
R. G. Hennig, T. J. Lenosky, D. R. Trinkle, S. P. Rudin, and J. W. Wilkins.
Phys. Rev. B **78**, 054121 (2008), doi://10.1103/PhysRevB.78.054121
11. *Lattice green function for extended defect calculations: Computation and error estimation with long-range forces*.
D. R. Trinkle.
Phys. Rev. B **78**, 014110 (2008), doi://10.1103/PhysRevB.78.014110

10. *Prediction of dislocation cores in aluminum from density functional theory*.
C. Woodward, D. R. Trinkle, L. G. Hector, Jr., and D. L. Olmsted.
Phys. Rev. Lett. **100**, 045507 (2008), doi://10.1103/PhysRevLett.100.045507
9. *Contribution to size effect of yield strength from the stochastics of dislocation source lengths in finite samples*.
T. A. Parthasarathy, S. I. Rao, D. M. Dimiduk, M. D. Uchic, and D. R. Trinkle.
Scripta mater. **56**, 313–316 (2007), doi://10.1016/j.scriptamat.2006.09.016
8. *Lattice and elastic constants of titanium-niobium monoborides containing aluminum and vanadium*.
D. R. Trinkle.
Scripta mater. **56**, 273–276 (2007), doi://10.1016/j.scriptamat.2006.10.030
7. *An empirical tight-binding model for titanium phase transformations*.
D. R. Trinkle, M. D. Jones, R. G. Hennig, S. P. Rudin, R. C. Albers, and J. W. Wilkins.
Phys. Rev. B **73**, 094123 (2006), doi://10.1103/PhysRevB.73.094123
6. *The chemistry of deformation: How solutes soften pure metals*.
D. R. Trinkle and C. Woodward.
Science **310**, 1665–1667 (2005), doi://10.1126/science.1118616
5. *Systematic pathway generation and sorting in martensitic transformations: Titanium alpha to omega*.
D. R. Trinkle, D. M. Hatch, H. T. Stokes, R. G. Hennig, and R. C. Albers.
Phys. Rev. B **72**, 014105 (2005), doi://10.1103/PhysRevB.72.014105
4. *Impurities block the alpha to omega martensitic transformation in Titanium*.
R. G. Hennig, D. R. Trinkle, J. Bouchet, S. G. Srinivasan, R. C. Albers, and J. W. Wilkins.
Nat. Mater. **4**, 129–133 (2005), doi://10.1038/nmat1292
3. *A new mechanism for the alpha to omega martensitic transformation in pure Titanium*.
D. R. Trinkle, R. G. Hennig, S. G. Srinivasan, D. M. Hatch, M. D. Jones, H. T. Stokes, R. C. Albers, and J. W. Wilkins.
Phys. Rev. Lett. **91**(2), 025701 (2003), doi://10.1103/PhysRevLett.91.025701
2. *Shock induced α-ω transition in titanium*.
C. W. Greeff, D. R. Trinkle, and R. C. Albers.
J. Appl. Phys. **90**(5), 2221–2226 (2001), doi://10.1063/1.1389334
1. *Bound states in waveguides and bent quantum wires*.
J. P. Carini, J. T. Londergan, D. P. Murdock, D. Trinkle, and C. S. Yung.
Phys. Rev. B **55**, 9842–9851 (1997), doi://10.1103/PhysRevB.55.9842

Submitted Papers

1. *Effect of solutes on the lattice parameters and elastic stiffness coefficients of body-centered tetragonal Fe*.
M. R. Fellinger, L. G. Hector, Jr., and D. R. Trinkle, (under review, Comp. Mater. Sci.) (2018)

Open-source Software and Databases

10. Software: Onsager, D. R. Trinkle.
http://dallastrinkle.github.io/Onsager, v1.2.2 (2017), doi://10.5281/zenodo.494987
9. Software: Bader Integration, D. R. Trinkle and M. Yu.
https://github.com/DallasTrinkle/BaderIntegration, v1.01 (2015), doi://10.5281/zenodo.18776

8. Database: *Data citation: Solute transport database in mg using ab initio and exact diffusion theory*, R. Agarwal and D. R. Trinkle (2017).
   dx.doi.org/10.18126/M20G83
7. Database: *Data citation: Mechanical properties and phase stability of monoborides using density functional theory calculations*, H. Kim and D. R. Trinkle (2017).
   dx.doi.org/10.18126/M24S3J
6. Database: *Data citation: Fitting database entries for a modified embedded atom method potential for interstitial oxygen in titanium*, D. R. Trinkle and P. Zhang (2016).
   hdl.handle.net/11256/782
5. Database: *Data citation: Light element diffusion in Mg using first principles calculations: Anisotropy and elastodiffusion*, R. Agarwal and D. R. Trinkle (2016).
   hdl.handle.net/11256/694
4. Database: *Data citation: Ab initio calculations of the lattice parameter and elastic stiffness coefficients of bcc Fe with solutes*, M. R. Fellinger, L. G. Hector, Jr., and D. R. Trinkle (2016).
   hdl.handle.net/11256/671
   Data files for ab initio calculations of the lattice parameter and elastic stiffness coefficients of BCC Fe with solutes.
   M. R. Fellinger, L. G. Hector, Jr., and D. R. Trinkle.
   Data in Brief **10**, 147–150 (2017), doi://10.1016/j.dib.2016.11.092.
   Database: hdl.handle.net/11256/671
3. Database: *Data citation: Diffusion of Si impurities in Ni under stress: A first-principles study*, T. Garnier, V. R. Manga, P. Bellon, and D. R. Trinkle (2014).
   hdl.handle.net/11115/239
2. Database: *Data citation: Solute effect on oxygen diffusion in α-titanium*, H. H. Wu and D. R. Trinkle (2013).
   hdl.handle.net/11115/125
1. Database: *Dallas R. Trinkle Research Group Magnesium Database*, J. A. Yasi and D. R. Trinkle (2013).
   magnesium.matse.illinois.edu

Conference Proceedings and Other Publications

7. *Applying for computational time on NSF's* TeraGrid*—the world's largest cyberinfrastructure supporting open research*.
   K. Thornton, D. R. Trinkle, and R. G. Hennig.
   JOM **62**, 17–18 (2010), doi://10.1007/s11837-010-0042-6
6. *Hydrogen trapping in dislocations in palladium at low temperature: Results from inelastic neutron scattering and advanced computations*.
   B. J. Heuser, H. Ju, D. R. Trinkle, and T. J. Udovic.
   In *Effects of Hydrogen on Materials*, 2008 International Hydrogen Conference, 464–468 (2009)
5. *Ab-initio molecular dynamics simulations of molten Ni-based superalloys*.
   M. Asta, D. R. Trinkle, and C. Woodward.
   In *2007 High Performance Computing User's Group Conference*, 147–152 (IEEE Computing Society, Los Alamitos, CA, 2007)
4. *Ab-initio molecular dynamics simulations of molten Ni-based superalloys*.
   M. Asta, D. R. Trinkle, and C. Woodward.
   In *2006 High Performance Computing User's Group Conference*, 177–181 (IEEE Computing Society, Los Alamitos, CA, 2007)

3. *Alpha-omega transition in Ti: Equation of state and kinetics*.
C. W. Greeff, D. R. Trinkle, and R. C. Albers.
AIP Conference Proceedings **620**(1), 225–228 (2002)
2. *Actinide electronic structure and atomic forces*.
R. C. Albers, S. P. Rudin, D. R. Trinkle, and M. D. Jones.
AIP Conference Proceedings **532**, 412–413 (2000)
1. *Amazing magnetic moments*.
R. Singleton, D. Trinkle, and T. Toepker.
Phys. Teach. **35**(2), 122–125 (1997), doi://10.1119/1.2344615

Invited Talks

—2017

83. *Exact theory of vacancy-mediated solute transport in magnesium.*
EuroMat 2017: European Congress and Exhibition on Advanced Materials and Processes. Thessaloniki, Greece, September 18, 2017.
82. *Dislocation cores from first principles: Ni and Ni_3Al for superalloys.*
US National Congress on Computational Mechanics (USNCCM14). Montreal, Canada, July 17, 2017.
81. *Dislocation cores and defect interactions from first principles: Current state of the art and new challenges.*
"Density Functional Theory and Beyond: Analysis and Computation" workshop, Mathematics Institute of the University of Warwick. Warwick, England, July 3, 2017.
80. *Automated Green function calculation of dilute solute diffusivity.*
DIMAT 2017: International Conference on Diffusion in Materials. Haifa, Israel, May 7, 2017.
79. *Exact theory of vacancy-mediated solute transport in magnesium.*
Magnesium Workshop: Alloys and Lightweight Structural Systems, Johns Hopkins University. Baltimore, Maryland, April 3, 2017.
78. *Dislocation core structures in Ni-based superalloys computed using density functional theory based flexible boundary condition approach.*
Modeling and Simulation of Superalloys International Workshop, Ruhr-Universität. Bochum, Germany, March 29, 2017.
77. *Computing mass transport in crystals: Theory, computation, and applications.*
Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany, March 27, 2017.
76. *Computing mass transport in crystals: Theory, computation, and applications.*
Materials Science and Engineering Seminar, Univ. California, Berkeley. February 24, 2017.

—2016

75. *Computing mass transport in crystals: Theory, computation, and applications.*
William Maxwell Reid Seminar, Univ. Kentucky. Lexington, KY, October 28, 2016.
74. *Solute interactions with dislocations in BCC Fe.*
CECAM meeting, Ab Initio Description of Iron and Steel. Ringsberg, Germany, October 3–7, 2016.
73. *Dislocation cores and defect interactions from first principles: Current state of the art and new challenges.*
Society for Engineering Science, 53rd Annual Technical Meeting. College Park, MD, October 2–5, 2016.

72. *Bridging timescales: Automating diffusivity calculations for interstitial and solute diffusion from first-principles.*
    Recent Advances in Computational Methods for Nanoscale Phenomena workshop. Ann Arbor, MI, August 29–31, 2016.
71. *Database optimization for empirical interatomic potentials.*
    Annual Meeting of the Minerals, Metals & Materials Society, "Computational Methods for Uncertainty Quantification, Model Validation, and Stochastic Predictions" symposium. Nashville, TN, February 14–18, 2016.
70. *Hydrides and Hydrogen Pipe Diffusion in Palladium: First Principles, Kinetic Monte Carlo, and Neutron Scattering.*
    Annual Meeting of the Minerals, Metals & Materials Society, "Hume-Rothery" symposium. Nashville, TN, February 14–18, 2016.

—2015

69. *Automating Computation of Solute Diffusion.*
    Materials Science and Technology Meeting, "Data and Tools for Materials Discovery and Design" symposium. Columbus, OH, October 4–8, 2015.
68. *First-principles computation of a stepped surface: TiO_2*
    Materials Science and Technology Meeting, "Deformation and Transitions at Grain Boundaries IV" symposium. Columbus, OH, October 4–8, 2015.
67. *Hydrides and Hydrogen Pipe Diffusion in Palladium: First Principles, Kinetic Monte Carlo, and Neutron Scattering.*
    Service de Recherches de Metallurgie Physique seminar, CEA/Saclay, September 14, 2015.
66. *Automating diffusivity calculations for interstitial and solute diffusion from first-principles.*
    2015 Psi-k Conference, San Sebastián / Donostia, Spain, September 7–10, 2015.
65. *Multiscale evolution of defects near a dislocation: Solutes and vacancies in nickel.*
    "Defects in Materials," Lake Arrowhead reunion program. Institute for Pure and Applied Mathematics, UCLA, June 8, 2015.
64. *Light interstitial diffusion in magnesium.*
    NIST Diffusion workshop, Gaithersburg, MD, May 14–15, 2015.
63. *Evolution of defects near a dislocation: Solutes and vacancies in nickel.*
    Annual Meeting of the Minerals, Metals & Materials Society, "Computational Thermodynamics and Kinetics" symposium. Orlando, FL, March 15–19, 2015.

—2014

62. *Forming nanoprecipitates at dislocations: Hydrides in Pd and Silicides in Ni.*
    Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany, November 5, 2014.
61. *Stress and irradiation effects on solute diffusion to dislocations.*
    Multiscale Modeling of Materials Meeting, Berkeley, CA, October 6, 2014.
60. *Lattice Green function calculations in the presence of a dislocation*
    "Multiscale Models of Crystal Defects" program, Banff International Research Station for Mathematical Innovation and Discovery, September 21, 2014.
59. *Hydrogen Pipe Diffusion in Palladium: First Principles, Kinetic Monte Carlo, and Experiments*
    14^{th} International Symposium on Metal-Hydrogen Systems, Univ. Salford, Manchester, UK, July 25, 2014.
58. *Lattice Green function calculations in the presence of a dislocation*
    "Defects in Materials," Lake Arrowhead reunion program. Institute for Pure and Applied Mathematics, UCLA, June 9, 2014.

57. *Metal solute-oxygen interaction in titanium for changes in oxygen diffusivity*
NIST Diffusion workshop, Gaithersburg, MD, April 28–29, 2014.
56. *Forming nanoprecipitates at dislocations: Hydrides in Pd and Silicides in Ni.*
Spring Meeting of the Materials Research Society, San Francisco, CA, April 21–25, 2014.
55. *Stress and Irradiation Effects on Solute Diffusion to Dislocations.*
Annual Meeting of the American Chemical Society, "Radiation Hardened Materials for Accelerators, Reactors and Spacecraft" symposium. Dallas, TX, March 16–20, 2014.
54. *Deformation of Magnesium from First Principles.*
2nd ESISM Workshop in Kyoto, "Fundamental Issues of Structural Materials." Kyoto, Japan, March 11–12, 2014.
53. *Density-functional theory methods for interfaces: Lattice Greens Function and Energy Density Methods.*
Annual Meeting of the Minerals, Metals & Materials Society, "Mechanical Behavior Related to Interface Physics II" symposium. San Diego, CA, February 16–20, 2014.

—2013

52. *Interfaces in HCP Ti: twinning, transformation, oxygen.*
Materials Science and Technology Meeting, "Deformation and Transitions at Grain Boundaries III" symposium. Montreal, Canada, October 28–31, 2013.
51. *Dislocations with first principles: From defects to material behavior in magnesium.*
Computational Science and Engineering, Fall Seminar, Univ. Illinois, Urbana-Champaign, October 23, 2013.
50. *First principles modeling of titanium: oxygen, dislocations, and boundaries.*
Keynote lecture; Pacific Rim International Congress on Advanced Materials and Processing (PRICM-8), Light Metals and Alloys symposium, Waikoloa, Hawaii, August 4–9, 2013.
49. *Energy Density Method and Bader Integration for Defect Energies.*
International Symposium on Atomistic Modeling for Mechanics and Multiphysics of Materials (ISAM^4 2013), Tokyo, Japan, July 22, 2013.
48. *Deformation in magnesium from first-principles.*
Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany, July 10, 2013.
47. *Beyond binaries: Solid solution strengthening and softening in magnesium.*
Magnesium Workshop Madrid 2013, Madrid, Spain, May 21–24, 2013.
46. *Stress-induced anisotropic diffusion in alloys: Complex Si solute flow near a dislocation core in Ni.*
NIST Diffusion workshop, Gaithersburg, MD, May 9–10, 2013.
45. *Predicting strength and cross-slip of magnesium alloys: First-principles, solute distribution, and deformation.*
Annual Meeting of the Minerals, Metals & Materials Society, "Modeling and Experimental Validation of Multiscale Mechanical Behavior from Atomic Scale to Macro Scale" symposium. San Antonio, TX, March 4–March 7, 2013.

—2012

44. *Solute diffusion under stress around dislocations: Si in Ni.*
Workshop on "Simulation of Complex Microstructure Pathways for Alloy Design." McMaster University, Hamilton, CA, November 29–30, 2012.
43. *Deformation in magnesium from first-principles.*
    (a) Physics Colloquium, California State Univ., Northridge, November 9, 2012.

(b) Materials Science and Engineering Colloquium, Univ. British-Columbia, November 6, 2012.
(c) Physics Colloquium, Arizona State Univ., November 5, 2012.
(d) Materials Science and Engineering Colloquium, Ohio State Univ., October 5, 2012.
(e) Materials Science and Engineering Colloquium, Univ. Florida, September 19, 2012.

42. *Dislocation cores and defect interactions from first principles: Current state of the art and new challenges.*
"Atomistic and Mesoscale Modeling of Materials Defects" workshop. Institute for Pure and Applied Mathematics, UCLA, October 22, 2012.
41. *Solute diffusion to dislocations under irradiation: Si in Ni.*
Materials Science and Technology Meeting, "Materials Development for Nuclear Applications and Extreme Environments" symposium. Pittsburgh, PA, October 7–11, 2012.
40. *From dislocation/solute interactions and solute distribution to deformation in magnesium.*
9th International Conference on Magnesium Alloys and their Applications. Vancouver, BC, Canada, July 8–12, 2012.
39. *Deformation in magnesium from first-principles.*
(a) Materials Science and Engineering Colloquium, Los Alamos National Laboratory, June 19, 2012.
(b) NIST Metallurgy Colloquium, July 6, 2012.
38. *The Challenge of Multicomponent Systems: Atomistics, Thermodynamics and Kinetics.*
NSF Workshop on Emerging Research Areas in the Science of Metals and Metallic Nanostructures. Univ. California, Santa Barbara, June 13–14, 2012.
37. *Atomic-scale modeling and data.*
NIST "Materials Genome Initiative Workshop on Building the Materials Innovation Infrastructure: Data and Standards." U.S. Department of Commerce, Washington, D.C., May 14–15, 2012.
36. *Deformation in magnesium from first-principles.*
Annual Meeting of the Minerals, Metals & Materials Society (TMS), "Phase Transformations and Deformation in Magnesium Alloys" symposium. Orlando, FL, March 11–March 15, 2012.
35. *First Principles Modeling of Dislocation/Twin Boundary Interactions in Titanium.*
International Conference on Plasticity. Puerto Rico, January 3–8, 2012.

—2011

34. *Deformation in magnesium from first-principles.*
U.S. Army Research Laboratory speaker series on Integrated Computational Materials Engineering, Aberdeen Proving Ground, MD, November 16, 2011.
33. *First-principles predictions of dislocation/solute interactions: Rare earths in magnesium.*
MagNET Research Network Workshop, "Rare Earth Elements in Magnesium Alloys." CANMET Facility, Hamilton, Ontario, November 7–8, 2011.
32. *Interactions of dislocations and twin boundaries in titanium with first-principles.*
Materials Science and Technology Meeting, "Deformation and Transitions at Grain Boundaries" symposium. Columbus, OH, October 16–20, 2011.
31. *Dislocations with first principles: From defects to material behavior in magnesium.*
Materials Science and Engineering Colloquium, Massachusetts Institute of Technology, October 13, 2011.

30. *First principles modeling of dislocations for magnesium alloys.*
    Keynote lecture; NSF Workshop on Magnesium Science and Technology, Arlington, VA, May 19–20, 2011.
29. *Dislocations with first principles: From defects to material behavior.*
    (a) Materials Science and Engineering Colloquium, Univ. Michigan, April 15, 2011.
    (b) Materials Science and Engineering Colloquium, Cornell University, April 21, 2011.
28. *Formation of hydrogen Cottrell atmosphere in palladium: Theory and measurement from inelastic neutron scattering.*
    Annual Meeting of the Minerals, Metals & Materials Society (TMS), "Hydrogen Storage in Materials: Theory and Experiment" symposium. San Diego, CA, February 27–March 3, 2011.
27. *Predicting Mg strength from first-principles: Solid-solution strengthening, softening, and cross-slip.*
    Keynote lecture; Annual Meeting of the Minerals, Metals & Materials Society (TMS), "Magnesium Technology 2011" symposium. San Diego, CA, February 27–March 3, 2011.
26. *Dislocations with first principles: From defects to material behavior.*
    (a) Materials Science and Engineering Colloquium, Univ. California, Berkeley, February 24, 2011.
    (b) Lawrence Livermore National Laboratory, February 25, 2011.

—2010

25. *Dislocations from first principles: Connecting defects to macroscale behavior in real materials.*
    (a) Mechanical, Aerospace, and Nuclear Engineering Colloquium, Rensselaer Polytechnic Institute, November 10, 2010.
    (b) Materials Science and Engineering Colloquium, California Institute of Technology, December 8.
    (c) Physics and Theory Colloquium, Los Alamos National Laboratory, December 9, 2010.

—2009

24. *Point, line, and planar defects and interactions using electronic structure methods.*
    CAMM meeting, "Possibilities and Limitations of Characterization and Modeling Solid/Solid Interfaces." Bernkastel-Kues, Germany, May 17–20, 2009.
23. *Palladium-hydrogen interaction in dislocations: Trapping and diffusion.*
    Annual Meeting of the Minerals, Metals & Materials Society (TMS), "Computational Thermodynamics and Kinetics" symposium. San Francisco, CA, February 15–20, 2009.
22. *Interface mobility for Ti alpha to omega transformation.*
    Annual Meeting of the Minerals, Metals & Materials Society (TMS), "Transformations Under Extreme Conditions" symposium. San Francisco, CA, February 15–20, 2009.
21. *Chemical short-range ordering in liquid-phase Ni alloys.*
    Annual Meeting of the Minerals, Metals & Materials Society (TMS), "Advanced Characterization and Modeling of Phase Transformations in Metals" symposium. San Francisco, CA, February 15–20, 2009.
20. *Electronic structure in dislocation modeling: Dislocation/solute interactions in Mo, Al, and Mg.*
    Joint Materials/Solid Mechanics Seminar Series, Brown Univ., January 30, 2009.
19. *Dislocation/solute interactions via first-principles for modeling strength of materials: Mo, Al, Mg.*
    International Conference on Plasticity. St. Thomas, January 3–8, 2009.

—2008

18. *First-principles calculation of dislocation/solute interaction: Solid-solution softening, dynamic strain-aging, and hydrogen trapping.*
    General Motors Research and Development, April 24, 2008.
17. *Electronic structure for dislocation/defect interactions.*
    Japan Institute of Metals Annual Meeting, Tokyo, Japan, March 28, 2008.

—2007

16. *First-principles calculation of dislocation/solute interaction: Solid-solution softening, dynamic strain-aging, and hydrogen trapping.*
    Materials Science and Engineering, Univ. Wisconsin, December 14, 2007.
15. *Chemistry of deformation: Solid-solution softening from first-principles to dislocation mobility.*
    Service de Recherches de Metallurgie Physique seminar, CEA/Saclay, June 26, 2007.
14. *Implementing flexible-boundary conditions and computing the lattice Green function.*
    Service de Recherches de Metallurgie Physique, Dislocation simulation workshop, CEA/Saclay, June 21, 2007.
13. *Density-functional theory, flexible-boundary conditions, and predicting dislocation-core structures.*
    Service de Recherches de Metallurgie Physique, Dislocation simulation workshop, CEA/Saclay, June 21, 2007.
12. *Material strength from first principles: Electronic structure and the solute/dislocation interaction.*
    Electronic Structure Workshop, North Carolina State University, June 12–15, 2007.
11. *Chemistry of deformation: From atomic bonding to dislocations to strength.*
    Joint Metallurgical Engineering and Material Science & Engineering graduate seminar, University of Utah, March 28, 2007.
10. *Chemistry of deformation: Solid-solution softening from first-principles to dislocation mobility.*
    Annual Meeting of the Minerals, Metals & Materials Society (TMS), "Plasticity from the Atomic Scale to Constitutive Laws" symposium. Orlando, FL, February 25–March 1, 2007.
9. *Martensitic alpha to omega in titanium: Atomic pathway and impurity effects.*
    Annual Meeting of the Minerals, Metals & Materials Society (TMS), "Fundamentals of Shape Memory and Related Transitions" symposium. Orlando, FL, February 25–March 1, 2007.

—2006

8. *The simulation of material deformation.*
    Physics in Careers seminar, Xavier University, October 20, 2006.
7. *The chemistry of deformation.*
    (a) Materials Science and Engineering colloquium, Univ. Illinois, Urbana-Champaign, January 23, 2006.
    (b) Mechanical Engineering seminar, Johns Hopkins University, February 7, 2006.
    (c) Materials Science and Engineering seminar, Northwestern University, March 1, 2006.

—2005

6. *Alpha to omega in titanium alloys: Martensitic phase transitions at the atomic length scale.*
    Materials Science and Technology, "Modeling and Simulation of Titanium Technology: Theory and Practices" symposium. Pittsburgh, PA, September 25–28, 2005.

5. *Martensitic phase transitions at the atomic length scale: Titanium alpha to omega.*
   March Meeting of the American Physical Society, Los Angeles, March 21–25, 2005.

—2003

4. *Atomistic mechanisms of the martensitic titanium hcp to omega phase transition.*
   Air Force Research Laboratory, Wright-Patterson AFB, August 20, 2003.
3. *Atomistic mechanisms of martensitic phase transformations: Titanium hcp to omega.*
   Electronic Structure Workshop, University of Minnesota, May 17–19, 2003.

—2001

2. *Investigating transition pathways with symmetry analysis and the nudged-elastic band method.*
   Condensed Matter seminar, Brigham Young University, October 18, 2001.

—1999

1. *Total energy and elastic properties of titanium via tight-binding.*
   Condensed Matter seminar, University of Cincinnati, July 14, 1999.

Conference Contributions

29. *Ab initio kinetic Monte Carlo study of hydrogen pipe diffusion.*
    2013 Gordon Research Conference on Hydrogen-Metal Systems, July 14.
28. *High-throughput solute interaction for deformation in magnesium from first-principles.*
    2012 Fall Meeting of the Materials Research Society, Materials Informatics Symposium, Boston, November 25.
27. *Predicting single crystal flow stress for magnesium alloys from first principles dislocation/solute interactions and solute distribution.*
    2012 Multiscale Modeling of Materials Meeting, Singapore, October 15, 2012.
26. *First principles dislocation/solute interactions and deformation in magnesium alloys.*
    2012 Dislocations, Budapest, Hungary, August 27, 2012.
25. *Interfacial reconstruction of Au/TiO_2 from ab initio.*
    2012 Annual Meeting of the Minerals, Metals & Materials Society (TMS), "Solid-State Interfaces II: Toward an Atomistic-Scale Understanding of Structure, Properties, and Behavior through Theory and Experiment" symposium. Orlando, FL, March 11–March 15.
24. *Au/TiO_2 interfacial reconstruction stability from ab initio.*
    2011 Materials Science and Technology Meeting, "Interfaces, Grain Boundaries and Surfaces from Atomistic and Macroscopic Approaches—Fundamental and Engineering Issues" symposium. Columbus, OH, October 16–20.
23. *Fundamentals of hydrogen and hydride formation at defects in palladium: First-principles prediction and inelastic neutron scattering measurements.*
    2011 Spring Meeting of the Materials Research Society, San Francisco, April 23–27.
22. *First-principles calculation of dislocation/solute interactions and modeling of strength in Mg.*
    Multiscale Materials Modeling 2010, Freiburg, Germany, October 4–8.
21. *Ab initio modeling to improve oxygen tolerance of Ti alloys.*
    Multiscale Materials Modeling 2010, Freiburg, Germany, October 4–8.
20. *H trapping and diffusion in Pd dislocation cores.*
    2008 Fall Meeting of the Materials Research Society, Boston, December 1–5.
19. *Ab initio calculation of H in Pd dislocation core.*
    2007 Fall Meeting of the Materials Research Society, Boston, November 26–30.

18. *New quantitative analysis explains softening of pure metals by solutes.*
    2006 Annual Meeting of the Minerals, Metals & Materials Society (TMS), San Antonio, March 12–16.
17. *Quantitative modeling of solid-solution softening in bcc Mo at the atomistic scale.*
    2005 Fall Meeting of the Materials Research Society, Boston, November 28–December 2.
16. *Intrinsic solid-solution softening in bcc Mo from dislocation-solute interactions.*
    2005 March Meeting of the American Physical Society, Los Angeles, March 21–25.
15. *Solid-solution softening trends in bcc Mo by first principles.*
    2005 Annual Meeting of the Minerals, Metals & Materials Society (TMS), San Francisco, February 14–17.
14. *Solid-solution softening in bcc molybdenum from first principles.*
    2004 MS&T Annual Meeting, New Orleans, LA, September 26–30.
13. *The lattice Green function for phonons: Decoupling short and long range contributions.*
    2004 Electronic Structure Workshop, New Brunswick, NJ, May 27–30. (poster)
12. *Impurities block the alpha to omega martensitic transformation in titanium.*
    2004 Annual Meeting of the Minerals, Metals & Materials Society (TMS), Charlotte, March 15–18.
11. *Inhomogeneous mechanism for the hcp to omega martensitic transformation in pure titanium.*
    2003 March Meeting of the American Physical Society, Austin, March 3–7.
10. *A new mechanism for hcp-omega transformation in pure titanium.*
    2003 Annual Meeting of the Minerals, Metals & Materials Society (TMS), San Diego, March 2–6.
9. *The mechanism of the titanium hcp to omega transformation.*
    2002 Electronic Structure Workshop, Berkeley, June 5–8. (poster)
8. *Titanium hcp to omega transformation with oxygen impurities.*
    2002 March Meeting of the American Physical Society, Indianapolis, March 18–22.
7. *Complete Titanium HCP to Omega Transformation Mechanism.*
    2002 March Meeting of the American Physical Society, Indianapolis, March 18–22.
6. *Modeling the hcp to omega phase transition in titanium.*
    2000 Psi-k Conference, Schwäbisch Gmünd, Germany, August 22–26. (poster)
5. *An improved tight-binding model for titanium.*
    2000 March Meeting of the American Physical Society, Minneapolis, March 20–24.
4. *Modeling the hcp to omega phase transition in titanium.*
    1999 Psi-k Workshop on Calculation of Material Properties, Trieste, Italy, August 9–18. (poster)
3. *Total energy and elastic properties of titanium via tight-binding.*
    1999 Electronic Structure Workshop, Urbana-Champaign, May 21–24. (poster)
2. *Interstitials on Si* {113} *surface.*
    1998 Electronic Structure Workshop, Philadelphia, May 29–31. (poster)
1. *Interstitials on Si* {113} *surface.*
    1998 March Meeting of the American Physical Society, Los Angeles, March 23–27.

Current Advisees

Abhinav Jain (Ph.D., 2012–present)
Ravi Agarwal (Ph.D., 2012–present)
Anne Marie Tan (Ph.D., 2012–present)
Hyojung Kim (Ph.D., 2013–present)
Yang Dan (Ph.D., 2016–present)
Josh Vita (Ph.D., 2017–present)
Soham Chattopadhyay (Ph.D., 2017–present)
Dr. Michael Fellinger (postdoc, 2013–present)
Lauren Smith (B.S., 2016–present)

Past Advisees

Min Yu (Ph.D., 2010; Coadvised with Prof. R. Martin, Physics) "Energy density method and its applications to defect energies."
Maryam Ghazisaeidi (Ph.D., 2011) "A first principles study of defects in Titanium: Interaction of twin boundaries with dislocations and oxygen interstitials."
Joseph A. Yasi (Ph.D., 2012) "Strength and ductility of Mg alloys from first-principles."
Henry W. Wu (Ph.D., 2013) "Oxygen diffusion through titanium and other HCP metals."
Pinchao Zhang (Ph.D., 2016) "Database optimization algorithm for empirical potentials."
Zebo Li (Ph.D., 2017) "Multi-scale investigation of vacancy-mediated diffusion of Si in Ni near an edge dislocation."
Emily Schiavone (Ph.D., 2017) "Ab initio modeling of hydrogen pipe diffusion in palladium."

Dr. Hadley Lawler (postdoc, 2009–2010)
Dr. Venkateswara Rao Manga (postdoc, 2010–2013)
Dr. Thomas Garnier (postdoc, 2013–2014)
Dr. Bora Lee (postdoc, 2013–2015)
Dr. Thomas Schuler (postdoc, 2015–2016)

Chanda Lowrance (B.S., 2009–2010)
Pandu Wisesa (B.S., 2011–2012)
Arvind Srikanth (B.S., 2011–2013)
Ah-Young Song (M.S., 2011–2013)

Delma Nieves Rivera (REU, Univ. Puerto Rico, Summer 2014)
Ellango Jothimurugesan (REU, Duke, Summer 2014)
Cal Williams (REU, Univ. Roanoke, Summer 2015)
Randall Pittman (REU, Univ. Roanoke, Summer 2015)