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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

2006-	Assistant Professor of Materials Science and Engineering, University of Illinois, Urbana-Champaign
2009-	Affiliated Assistant Professor of Nuclear, Plasma, and Radiological Engineering, University of Illinois, Urbana-Champaign
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

Xerox Faculty Research Award (2011)	<i>Univ. Illinois</i>
Early Career Fellow, Honorable Mention (2011)	<i>TMS</i>
Faculty Early Career Development Award (CAREER, 2009)	<i>NSF/CMMI</i>
3M Untenured Faculty Research Award (2008, 2009, 2010)	<i>3M</i>
Young Leader International Scholar Award (2008)	<i>TMS</i>
Young Leader Intern (Professional Development Award)	<i>TMS</i>
Structural Materials Division (2006)	
National Research Council Associate (2004-2006)	<i>Air Force Research Laboratory</i>
Fowler Fellow (1996-1998, 2000-2001)	<i>Ohio State University</i>

Professional Activities

Co-chair, 2011 Physical Metallurgy Gordon conference
Organizer, 2007-2011 ASM Materials Camp for high school teachers, UIUC
Organizer, 2011 Girls Learning About Materials summer camp for high school seniors, UIUC
Organizer, 2008 "Recent Developments in Electronic Structure Methods" workshop, UIUC
Organizer, 2006 "Recent Developments in Electronic Structure Methods" workshop, OSU
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
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.

TMS technical committees: Chemistry and Physics of Materials; Computational Materials Science and Engineering; Magnesium; High Temperature Alloys; Young Leaders

Current Research Grants

6. *Materials for Extreme Irradiation Environments*. Illinois MRL Cluster; DOE/BES.
5. *Surface and Interface Free Energies of Epitaxial Nanocrystals*. J. Zuo and D. R. Trinkle; NSF/DMR.
4. *Designing Oxygen-tolerant Titanium Alloys with First-principles*. D. R. Trinkle; Boeing.
3. *CAREER: First-Principles Modeling of Titanium-Oxygen-Solute Interaction: Materials Design for Improved Energy Efficiency*. D. R. Trinkle; NSF/CMMI.
2. *GOALI: Modeling solute effects in magnesium alloys: First-principles to predictive finite-element*. D. R. Trinkle and L. G. Hector, Jr.; NSF/CMMI.
1. *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.

Past Research Grants

1. *Heteroepitaxial metal nanostructure diffusion through collective slip*. J. Weaver and D. R. Trinkle; NSF/DMR (06/15/07–06/14/10).

Refereed Publications

30. *Au/TiO₂(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 H₂O 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

3. *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, (under review, Acta Mater.) (2011)
2. *Strong gold nanocrystal and support interactions on rutile (110) surfaces from interfacial reduction and bonding.*
S. Sivaramakrishnan, M. Yu, B. J. Pierce, M. E. Scarpelli, J. Wen, D. R. Trinkle, and J.-M. Zuo, (under review, Science) (2011)
1. *Investigation of defect recovery in deformed Pd: Correlation between positron lifetime, enhanced hydrogen solubility, and transmission electron microscopy analysis.*
H. Ju, B. J. Heuser, D. R. Trinkle, V. McCreary, J. Fenske, and I. M. Robertson, (under review, J. Phys. CM) (2011)

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

34. *Deformation in magnesium from first-principles.*
U.S. Army Research Laboratory speaker series on Integrated Computational Materials Engineering, Aberdeen Proving Ground, MD, Nov. 16, 2011.
33. *First-principles predictions of dislocation/solute interactions: Rare earths in magnesium.*
MagNET Research Network Workshop, "Rare Earth Elements in Magnesium Alloys." CAN-MET Facility, Hamilton, Ontario, Nov. 7–8, 2011.
32. *Interactions of dislocations and twin boundaries in titanium with first-principles.*
2011 Materials Science and Technology Meeting, "Deformation and Transitions at Grain Boundaries" symposium. Columbus, OH, Oct. 16–20.
31. *Dislocations with first principles: From defects to material behavior in magnesium.*
Materials Science and Engineering Colloquium, Massachusetts Institute of Technology, Oct. 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.*
2011 Annual Meeting of the Minerals, Metals & Materials Society, "Hydrogen Storage in Materials: Theory and Experiment" symposium. San Diego, CA, Feb. 27–Mar. 3.
27. *Predicting Mg strength from first-principles: Solid-solution strengthening, softening, and cross-slip.*
Keynote lecture; 2011 Annual Meeting of the Minerals, Metals & Materials Society, "Magnesium Technology 2011" symposium. San Diego, CA, Feb. 27–Mar. 3.
26. *Dislocations with first principles: From defects to material behavior.*
 - (a) Materials Science and Engineering Colloquium, Univ. California, Berkeley, Feb. 24, 2011.
 - (b) Lawrence Livermore National Laboratory, Feb. 25, 2011.
25. *Dislocations from first principles: Connecting defects to macroscale behavior in real materials.*
 - (a) Mechanical, Aerospace, and Nuclear Engineering Colloquium, Rensselaer Polytechnic Institute, Nov. 10, 2010.
 - (b) Materials Science and Engineering Colloquium, California Institute of Technology, Dec. 8, 2010.
 - (c) Physics and Theory Colloquium, Los Alamos National Laboratory, Dec. 9, 2010.
24. *Point, line, and planar defects and interactions using electronic structure methods.*
2009 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.*
2009 Annual Meeting of the Minerals, Metals & Materials Society, "Computational Thermodynamics and Kinetics" symposium. San Francisco, CA, Feb. 15–20.
22. *Interface mobility for Ti alpha to omega transformation.*
2009 Annual Meeting of the Minerals, Metals & Materials Society, "Transformations Under Extreme Conditions" symposium. San Francisco, CA, Feb. 15–20.
21. *Chemical short-range ordering in liquid-phase Ni alloys.*
2009 Annual Meeting of the Minerals, Metals & Materials Society, "Advanced Characterization and Modeling of Phase Transformations in Metals" symposium. San Francisco, CA, Feb. 15–20.
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.*
2009 International Conference on Plasticity. St. Thomas, Jan. 3–8.
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, March 28, 2008.
16. *First-principles calculation of dislocation/solute interaction: Solid-solution softening, dynamic strain-aging, and hydrogen trapping.*
Materials Science and Engineering, Univ. Wisconsin, Dec. 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.*
2007 Electronic Structure Workshop, North Carolina State University, June 12–15.
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.*
2007 Annual Meeting of the Minerals, Metals & Materials Society, “Plasticity from the Atomic Scale to Constitutive Laws” symposium. Orlando, FL, Feb. 25–Mar. 1.
9. *Martensitic alpha to omega in titanium: Atomic pathway and impurity effects.*
2007 Annual Meeting of the Minerals, Metals & Materials Society, “Fundamentals of Shape Memory and Related Transitions” symposium. Orlando, FL, Feb. 25–Mar. 1.
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, Jan. 23, 2006.
 - (b) Mechanical Engineering seminar, Johns Hopkins University, Feb. 7, 2006.
 - (c) Materials Science and Engineering seminar, Northwestern University, March 1, 2006.
6. *Alpha to omega in titanium alloys: Martensitic phase transitions at the atomic length scale.*
Materials Science and Technology 2005, “Modeling and Simulation of Titanium Technology: Theory and Practices” symposium. Pittsburgh, PA, Sept. 25–28, 2005.
5. *Martensitic phase transitions at the atomic length scale: Titanium alpha to omega.*
2005 March Meeting of the American Physical Society, Los Angeles, March 21–25.
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.*
2003 Electronic Structure Workshop, University of Minnesota, May 17–19.
2. *Investigating transition pathways with symmetry analysis and the nudged-elastic band method.*
Condensed Matter seminar, Brigham Young University, Oct. 18, 2001.
1. *Total energy and elastic properties of titanium via tight-binding.*
Condensed Matter seminar, University of Cincinnati, July 14, 1999.

Conference Contributions

24. *Au/TiO₂ 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, Oct. 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, Apr. 23–27.
22. *First-principles calculation of dislocation/solute interactions and modeling of strength in Mg.*
Multiscale Materials Modeling 2010, Freiburg, Germany, Oct. 4–8.
21. *Ab initio modeling to improve oxygen tolerance of Ti alloys.*
Multiscale Materials Modeling 2010, Freiburg, Germany, Oct. 4–8.
20. *H trapping and diffusion in Pd dislocation cores.*
2008 Fall Meeting of the Materials Research Society, Boston, Dec. 1–5.
19. *Ab initio calculation of H in Pd dislocation core.*
2007 Fall Meeting of the Materials Research Society, Boston, Nov. 26–30.
18. *New quantitative analysis explains softening of pure metals by solutes.*
2006 Annual Meeting of the Minerals, Metals & Materials Society, San Antonio, Mar. 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, Nov. 28–Dec. 2.
16. *Intrinsic solid-solution softening in bcc Mo from dislocation-solute interactions.*
2005 March Meeting of the American Physical Society, Los Angeles, Mar. 21–25.
15. *Solid-solution softening trends in bcc Mo by first principles.*
2005 Annual Meeting of the Minerals, Metals & Materials Society, San Francisco, Feb. 14–17.
14. *Solid-solution softening in bcc molybdenum from first principles.*
2004 MS&T Annual Meeting, New Orleans, LA, Sept. 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, 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, 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, Aug. 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, Aug. 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

Henry Wu (Ph.D., 2006–present)
Joseph Yasi (Ph.D., 2007–present)
Pinchao Zhang (Ph.D., 2008–present)
Emily Schiavone (Ph.D., 2010–present)
Zebo Li (Ph.D., 2011–present)
Ah-Young Song (Ph.D., 2011–present)

Dr. Venkateswara Rao Manga (postdoc, 2010–present)

Panda Wisesa (B.S., 2011–present)
Arvind Srikanth (B.S., 2011–present)

Past Advisees

Maryam Ghazisaeidi (Ph.D., 2011; “A first principles study of defects in Titanium: Interaction of twin boundaries with dislocations and oxygen interstitials.”)
Min Yu (Ph.D., 2010; “Energy density method and its applications to defect energies.” Coadvised with Prof. R. Martin, Physics)

Dr. Hadley Lawler (postdoc, 2009–2010)

Chanda Lowrance (B.S., 2009–2010)