

Dallas R. Trinkle

Curriculum Vitæ

University of Illinois, Urbana-Champaign
Materials Science and Engineering
1304 West Green Street
Urbana, IL 61801

Office: (217) 244-6519
Fax: (217) 333-2736
Email: dtrinkle@illinois.edu
URL: <http://dtrinkle.matse.illinois.edu>

Professional Preparation

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| 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

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| 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

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| Faculty Early Career Development Award (CAREER, 2009) | <i>NSF/CMMI</i> |
| 3M Untenured Faculty Research Award (2008, 2009) | <i>3M</i> |
| Young Leader International Scholar Award (2008) | <i>TMS</i> |
| Young Leader Intern (Professional Development Award) Structural Materials Division (2006) | <i>TMS</i> |
| 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
NSF TeraGrid Allocations Committee Reviewer (2008-present)
Organizer, 2010 TMS annual meeting "Stochastic Methods in Materials Research" symposium
Organizer, 2010 TMS annual meeting "Computational Thermodynamics and Kinetics" symposium
Organizer, 2008 "Recent Developments in Electronic Structure Methods" workshop, UIUC
Organizer, 2008 TMS annual meeting "Minerals, Metals & Materials under Pressure" symposium
Organizer, 2006 TMS annual meeting "Point Defects in Materials" symposium
Organizer, 2006 "Recent Developments in Electronic Structure Methods" workshop, OSU
Organizer, 2007, 2008, 2009 ASM Materials Camp for high school teachers, UIUC
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.
TMS Committees: Chemistry and Physics of Materials; Computational Materials Science and Engineering; High Temperature Alloys; Young Leaders

Current Research Grants

1. *Heteroepitaxial metal nanostructure diffusion through collective slip*. J. Weaver and D. R. Trinkle; NSF/DMR.
2. *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.
3. *GOALI: Modeling solute effects in magnesium alloys: First-principles to predictive finite-element*. D. R. Trinkle and L. G. Hector, Jr.; NSF/CMMI.
4. *CAREER: First-Principles Modeling of Titanium-Oxygen-Solute Interaction: Materials Design for Improved Energy Efficiency*. D. R. Trinkle; NSF/CMMI.

Refereed Publications

1. *Cu/Ag EAM Potential Optimized for Heteroepitaxial Diffusion from ab initio Data*. H. H. Wu and D. R. Trinkle. *Comp. Mater. Sci.* (accepted) (2009). [arXiv:0901.0861](https://arxiv.org/abs/0901.0861)
2. *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. *Modelling Simul. Mater. Sci. Eng.* **17**, 055012 (2009). [doi://10.1088/0965-0393/17/5/055012](https://doi.org/10.1088/0965-0393/17/5/055012)
3. *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](https://doi.org/10.1103/PhysRevE.79.037701)
4. *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](https://doi.org/10.1073/pnas.0806456105)
5. *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](https://doi.org/10.1103/PhysRevB.78.054121)
6. *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](https://doi.org/10.1103/PhysRevB.78.014110)
7. *Prediction of dislocation cores in aluminum from density functional theory*. C. Woodward, D. R. Trinkle, L. G. Hector, D. L. Olmsted. *Phys. Rev. Lett.* **100**, 045507 (2008). [doi://10.1103/PhysRevLett.100.045507](https://doi.org/10.1103/PhysRevLett.100.045507)
8. *Lattice and elastic constants of Ti-Nb monoborides containing Al and V*. D. R. Trinkle. *Scripta mater.* **56**, 273–276 (2007). [doi://10.1016/j.scriptamat.2006.10.030](https://doi.org/10.1016/j.scriptamat.2006.10.030)
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](https://doi.org/10.1016/j.scriptamat.2006.09.016)
10. *An empirical tight-binding model for titanium phase transformations*. D. R. Trinkle, M. D. Jones, R. G. Hennig, S. P. Rudin, R. C. Albers, J. W. Wilkins. *Phys. Rev. B* **73**, 094123 (2006). [doi://10.1103/PhysRevB.73.094123](https://doi.org/10.1103/PhysRevB.73.094123)
11. *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](https://doi.org/10.1126/science.1118616)

12. *Systematic pathway generation and sorting in martensitic transformations: Titanium alpha to omega.*
D. R. Trinkle, D. M. Hatch, H. T. Stokes, R. G. Hennig, R. C. Albers.
Phys. Rev. B **72**, 014105 (2005). doi://10.1103/PhysRevB.72.014105
13. *Impurities block the alpha to omega martensitic transformation in titanium.*
R. G. Hennig, D. R. Trinkle, J. Bouchet, S. G. Srinivasan, R. C. Albers, J. W. Wilkins.
Nature Materials **4**(2), 129–133 (2005). doi://10.1038/nmat1292
14. *A new mechanism for the alpha to omega martensitic transformation in pure titanium.*
D. R. Trinkle, R. G. Hennig, S. G. Srivilliputhur, D. M. Hatch, H. T. Stokes, M. D. Jones, R. C. Albers, J. W. Wilkins.
Phys. Rev. Lett. **91**, 025701 (2003). doi://10.1103/PhysRevLett.91.025701
15. *Shock-induced $\alpha - \omega$ transition in titanium.*
C. W. Greeff, D. R. Trinkle, R. C. Albers.
J. Appl. Phys. **90**, 2221–2226 (2001). doi://10.1063/1.1389334
16. *Bound states in waveguides and bent quantum wires.*
J. P. Carini, J. T. Londergan, D. P. Murdock, D. Trinkle, C. S. Yung.
Phys. Rev. B **55**, 9842–9851 (1997). doi://10.1103/PhysRevB.55.9842

Submitted Papers

1. *Island Shape Controls Magic-Size Effect for Heteroepitaxial Diffusion.*
H. H. Wu, A. W. Signor and D. R. Trinkle. arXiv:0908.3006 (2009).

Conference Proceedings

1. *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.
Effects of Hydrogen on Materials (2008 International Hydrogen Conference) 464-468. (2009).
2. *Ab-Initio Molecular Dynamics Simulations of Molten Ni-Based Superalloys.*
M. Asta, D. R. Trinkle and C. Woodward.
Proceedings of the 2007 High Performance Computing User's Group Conference (IEEE Computing Society, Los Alamitos, CA) 147-152. (2007).
3. *Ab-Initio Molecular Dynamics Simulations of Molten Ni-Based Superalloys.*
M. Asta, D. R. Trinkle and C. Woodward.
Proceedings of the 2006 High Performance Computing User's Group Conference (IEEE Computing Society, Los Alamitos, CA) 177-181. (2007).
4. *Alpha-omega Transition in Ti: Equation of State and Kinetics*
C. W. Greeff, D. R. Trinkle, and R. C. Albers.
AIP Conference Proceedings **620**, pt.1, 225–8 (2002).
5. *Actinide Electronic Structure and Atomic Forces*
R. C. Albers, S. P. Rudin, D. R. Trinkle, and M. D. Jones.
AIP Conference Proceedings **532**, 412–3 (2000).

Invited Talks

1. *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.

2. *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.
3. *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.
4. *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.
5. *Electronic structure in dislocation modeling: Dislocation/solute interactions in Mo, Al, and Mg.*
Joint Materials/Solid Mechanics Seminar Series, Brown Univ., January 30, 2009.
6. *Dislocation/solute interactions via first-principles for modeling strength of materials: Mo, Al, Mg.*
2009 International Conference on Plasticity. St. Thomas, Jan. 3–8.
7. *First-principles calculation of dislocation/solute interaction: Solid-solution softening, dynamic strain-aging, and hydrogen trapping.*
General Motors Research and Development, April 24, 2008.
8. *Electronic structure for dislocation/defect interactions.*
Japan Institute of Metals Annual Meeting, Tokyo, March 28, 2008.
9. *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.
10. *Chemistry of deformation: Solid-solution softening from first-principles to dislocation mobility.*
Service de Recherches de Metallurgie Physique seminar, CEA/Saclay, June 26, 2007.
11. *Implementing flexible-boundary conditions and computing the lattice Green function.*
Service de Recherches de Metallurgie Physique, Dislocation simulation workshop, CEA/Saclay, June 21, 2007.
12. *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.
13. *Material strength from first principles: Electronic structure and the solute/dislocation interaction.*
2007 Electronic Structure Workshop, North Carolina State University, June 12–15.
14. *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.
15. *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.
16. *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.
17. *The simulation of material deformation.*
Physics in Careers seminar, Xavier University, October 20, 2006.
18. *The chemistry of deformation.*
Materials Science and Engineering seminar, Northwestern University, March 1, 2006.
Mechanical Engineering seminar, Johns Hopkins University, Feb. 7, 2006.
Materials Science and Engineering colloquium, Univ. Illinois, Urbana-Champaign, Jan. 23, 2006.

19. *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.
20. *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.
21. *Atomistic mechanisms of martensitic phase transformations: Titanium hcp to omega.* 2003 Electronic Structure Workshop, University of Minnesota, May 17–19.
22. *Investigating transition pathways with symmetry analysis and the nudged-elastic band method.* Condensed Matter seminar, Brigham Young University, Oct. 18, 2001.
23. *Total energy and elastic properties of titanium via tight-binding.* Condensed Matter seminar, University of Cincinnati, July 14, 1999.

Conference Contributions

1. *H trapping and diffusion in Pd dislocation cores.* 2008 Fall Meeting of the Materials Research Society, Boston, December 1–5.
2. *Ab initio calculation of H in Pd dislocation core.* 2007 Fall Meeting of the Materials Research Society, Boston, November 26–30.
3. *New quantitative analysis explains softening of pure metals by solutes.* 2006 Annual Meeting of the Minerals, Metals & Materials Society, San Antonio, March 12–16.
4. *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.
5. *Intrinsic solid-solution softening in bcc Mo from dislocation-solute interactions.* 2005 March Meeting of the American Physical Society, Los Angeles, March 21–25.
6. *Solid-solution softening trends in bcc Mo by first principles.* 2005 Annual Meeting of the Minerals, Metals & Materials Society, San Francisco, Feb. 14–17.
7. *Solid-solution softening in bcc molybdenum from first principles.* 2004 MS&T Annual Meeting, New Orleans, LA, Sept. 26–30.
8. *The lattice Green function for phonons: Decoupling short and long range contributions.* 2004 Electronic Structure Workshop, New Brunswick, NJ, May 27–30. (poster)
9. *Impurities block the alpha to omega martensitic transformation in titanium.* 2004 Annual Meeting of the Minerals, Metals & Materials Society, Charlotte, March 15–18.
10. *Inhomogeneous mechanism for the hcp to omega martensitic transformation in pure titanium.* 2003 March Meeting of the American Physical Society, Austin, March 3–7.
11. *A new mechanism for hcp-omega transformation in pure titanium.* 2003 Annual Meeting of the Minerals, Metals & Materials Society, San Diego, March 2–6.
12. *The mechanism of the titanium hcp to omega transformation.* 2002 Electronic Structure Workshop, Berkeley, June 5–8. (poster)
13. *Titanium hcp to omega transformation with oxygen impurities.* 2002 March Meeting of the American Physical Society, Indianapolis, March 18–22.
14. *Complete Titanium HCP to Omega Transformation Mechanism.* 2002 March Meeting of the American Physical Society, Indianapolis, March 18–22.
15. *Modeling the hcp to omega phase transition in titanium.* 2000 Psi-k Conference, Schwäbisch Gmünd, Germany, Aug. 22–26. (poster)
16. *An improved tight-binding model for titanium.* 2000 March Meeting of the American Physical Society, Minneapolis, March 20–24.

17. *Modeling the hcp to omega phase transition in titanium.*
1999 Psi-k Workshop on Calculation of Material Properties, Trieste, Italy, Aug. 9–18. (poster)
18. *Total energy and elastic properties of titanium via tight-binding.*
1999 Electronic Structure Workshop, Urbana-Champaign, May 21–24. (poster)
19. *Interstitials on Si {113} surface.*
1998 Electronic Structure Workshop, Philadelphia, May 29–31. (poster)
20. *Interstitials on Si {113} surface.*
1998 March Meeting of the American Physical Society, Los Angeles, March 23–27.

Past and Current Advisees

Henry Wu (Ph.D., 2006–present)

Joseph Yasi (Ph.D., 2007–present)

Maryam Ghazisaeidi (Ph.D., 2008–present)

Min Yu (Ph.D., 2008–present; coadvised with Prof. R. Martin, Physics)

PinChao Zhang (Ph.D., 2008–present)

Chanda Lowrance (B.S., 2009–present)

Dr. Hadley Lawler (postdoc, 2009–present)