John E. Klepeis

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EDUCATIONAL BACKGROUND

Stanford University, Stanford, California, 1985–1989

- Thesis advisor: Professor Walter A. Harrison
- Ph.D. in Applied Physics, 1989
- M.S. in Applied Physics, 1987

Cornell University, Ithaca, New York, 1981–1985

- B.S. with distinction in Applied and Engineering Physics, 1985

EMPLOYMENT EXPERIENCE

Lawrence Livermore National Laboratory, Livermore, California, 1989–present

- Theoretical and computational condensed matter physicist in Physics Directorate
- Promoted from postdoctoral to term appointment, 1992
- Promoted to career appointment, 1996
- Elevated to deputy group leader of Metals and Alloys Group, 2002
- Promoted to group leader of EOS and Materials Theory Group, 2006
- Providing broad technical expertise and scientific leadership in the areas of electronic structure and materials physics to multiple Laboratory programs
- Applying first-principles electronic structure methods to materials problems
- Managing existing actinide research programs and developing new programs
- Mentoring younger scientists and supervising students and visitors
- Performing administrative functions including performance appraisals, coordination with computer support personnel, and other institutional responsibilities

Universität Erlangen-Nürnberg, Erlangen, Germany, 1–2/1998, 4–5/1999, 6–7/2000

- Invited as visiting scientist in Lehrstuhl für Theoretische Festkörperphysik
- Gave lectures on full-potential linear muffin-tin orbital electronic structure method
- Studied mechanical and chemical bonding properties of platinum silicides

Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany, 10/1991–1/1992

- Invited as visiting scientist in Abteilung Theorie (theory department)
- Acquired expertise with full-potential linear muffin-tin orbital electronic structure code
- Studied metal overlayers on (110) surfaces of zinc-blende semiconductors

EMPLOYMENT EXPERIENCE (continued)

Stanford University, Stanford, California, 1985–1989

- Graduate research assistant in Applied Physics
- Performed tight-binding electronic structure calculations for semiconductor systems
- Gave guest lectures; Tutored students; Graded problem sets

HONORS

Outstanding Meeting Paper at the Materials Research Society Fall Meeting, 2006

Lawrence Livermore National Laboratory Distinguished Achievement Awards:

- Calculations of the effects of self-irradiation in actinide materials, 2004
- Research on the compressibility of osmium, 2002
- Contributions to high-pressure actinide phase diagrams, 2001
- High-pressure strength modeling for actinide materials, 2000
- High-pressure actinide elastic constant calculations, 1997

National Honor Societies:

- Phi Kappa Phi, Cornell University, 1985
- Tau Beta Pi, Cornell University, 1984

PROJECT MANAGEMENT

- Currently principal or co-principal investigator for five Advanced Simulation and Computing (ASC) projects on actinide equations-of-state, phase diagrams, strength modeling, optical properties, and self-irradiation, 1999–present
- Defend projects at invited briefings to external reviewers (see **Presentations**)
- Played key role in securing funding and developing new research program for BlueGene/L—currently the world's fastest supercomputer, 2004–present
- Successfully attracted funding for project on self-irradiation in actinides, 2003–present
- Contributed to successful funding of a theoretical and an experimental project to develop optical properties as a materials diagnostic under extreme conditions, 2003–present
- Principal investigator for theoretical portion of joint theory/experiment project on surfaces and interfaces funded by Basic Energy Sciences, 1997–2003

PROFESSIONAL ACTIVITIES

- Co-chair of actinide equation-of-state working group at JOWOG 32 Materials Meeting, Lawrence Livermore National Laboratory, Livermore, CA 2006
- Referee for journal articles submitted to Physical Review B, Physical Review Letters, Nature, Journal of Applied Physics, Applied Physics Letters, High Pressure Research, Materials Research Society Proceedings
- Referee for research proposals submitted to the Department of Energy
- Session chair at Materials Research Society Fall Meeting, Boston, MA 2005 and 2nd International Workshop on Orbital and Spin Magnetism of Actinides, Berkeley, CA 2002
- Member of American Physical Society, 1987–present

PUBLICATIONS

Refereed–Electronic Structure

1. **J. E. Klepeis**, *Introduction to first-principles electronic structure methods: Application to actinide materials*, J. Mater. Res. **21**, 2979 (2006).

2. L. X. Benedict, **J. E. Klepeis**, and F. H. Streitz, *Calculation of optical absorption in Al across the solid-to-liquid transition*, Phys. Rev. B **71**, 064103 (2005).

3. N. Franco, **J. E. Klepeis**, C. Bostedt, T. Van Buuren, C. Heske, O. Pankratov, T. A. Callcott, D. L. Ederer, and L. J. Terminello, *Experimental and theoretical electronic structure determination for PtSi*, Phys. Rev. B **68**, 045116 (2003).

4. **J. E. Klepeis**, O. Beckstein, O. Pankratov, and G. L. W. Hart, *Chemical bonding, elasticity, and valence force field models: A case study for α-Pt_2Si and PtSi*, Phys. Rev. B **64**, 155110 (2001).

5. O. Beckstein, **J. E. Klepeis**, G. L. W. Hart, and O. Pankratov, *First-principles elastic constants and electronic structure of α-Pt_2Si and PtSi*, Phys. Rev. B **63**, 134112 (2001).

6. A. K. McMahan and **J. E. Klepeis**, *Direct calculation of Slater-Koster parameters: Fourfold-coordinated silicon/boron phases*, Phys. Rev. B **56**, 12 250 (1997).

7. E. L. Shirley, L. J. Terminello, **J. E. Klepeis**, and F. J. Himpsel, *Detailed theoretical photoelectron angular distributions for LiF (100)*, Phys. Rev. B **53**, 10 296 (1996).

8. A. K. McMahan, **J. E. Klepeis**, M. van Schilfgaarde, and M. Methfessel, *Bonding in the molybdenum silicides*, Phys. Rev. B **50**, 10 742 (1994).

9. W. A. Harrison and **J. E. Klepeis**, *Dielectric screening in semiconductors*, Phys. Rev. B **37**, 864 (1988).

Refereed–High-Pressure Physics

1. A. Landa, **J. Klepeis**, P. Söderlind, I. Naumov, O. Velikokhatnyi, L. Vitos, and A. Ruban, *Fermi surface nesting and pre-martensitic softening in V and Nb at high pressures*, J. Phys.: Condens. Matter **18**, 5079 (2006).

2. H. Cynn, **J. E. Klepeis**, C.-S. Yoo, and D. A. Young, *Osmium has the lowest experimentally determined compressibility*, Phys. Rev. Lett. **88**, 135701 (2002).

3. T. W. Barbee III, A. K. McMahan, **J. E. Klepeis**, and M. van Schilfgaarde, *High-pressure boron hydride phases*, Phys. Rev. B **56**, 5148 (1997).

4. H. E. Lorenzana, **J. E. Klepeis**, M. J. Lipp, W. J. Evans, H. B. Radousky, and M. van Schilfgaarde, *High-pressure phases of PbF_2: A joint experimental and theoretical study*, Phys. Rev. B **56**, 543 (1997).

5. **J. E. Klepeis**, K. J. Schafer, T. W. Barbee III, and M. Ross, *Hydrogen-helium mixtures at megabar pressures: Implications for Jupiter and Saturn*, Science **254**, 986 (1991).

Refereed–Surfaces and Interfaces, Nanoscience

1. L. X. Benedict, A. Puzder, A. J. Williamson, J. C. Grossman, G. Galli, **J. E. Klepeis**, J.-Y. Raty, and O. Pankratov, *Calculation of optical absorption spectra of hydrogenated Si clusters: Bethe-Salpeter equation versus time-dependent local-density approximation*, Phys. Rev. B **68**, 085310 (2003).

2. L. Pizzagalli, G. Galli, **J. E. Klepeis**, and F. Gygi, *Structure and stability of germanium nanoparticles*, Phys. Rev. B **63**, 165324 (2001).

3. T. Wiell, **J. E. Klepeis**, P. Bennich, O. Björneholm, N. Wassdahl, and A. Nilsson, *Local aspects of the adsorbate–substrate chemical bond in N/Cu(100) and O/Cu(100)*, Phys. Rev. B **58**, 1655 (1998).

4. C. J. Wu and **J. E. Klepeis**, *The effect of Cl coverage on Si(100) surface reactivity: Implications for Cl etching of Si*, J. Phys.: Condens. Matter **10**, 4515 (1998).

5. C. J. Wu and **J. E. Klepeis**, *Halogen adsorption on transition-metal surfaces: A case study of Cl on Ta(110)*, Phys. Rev. B **55**, 10 848 (1997).

6. **J. E. Klepeis**, L. J. Terminello, and D. A. Lapiano-Smith, *Imaging of a surface state from clean Cu (001)*, Phys. Rev. B **53**, 16 035 (1996).

7. C. J. Wu, L. H. Yang, **J. E. Klepeis**, and C. Mailhiot, *Ab initio pseudopotential calculations of the atomic and electronic structure of the Ta (100) and (110) surfaces*, Phys. Rev. B **52**, 11 784 (1995).

8. T. Kendelewicz, **J. E. Klepeis**, J. C. Woicik, S. H. Southworth, C. Mailhiot, M. van Schilfgaarde, M. Methfessel, A. Herrera-Gomez, and K. E. Miyano, *Large-angle bond-rotation relaxation for CdTe (110)*, Phys. Rev. B **51**, 10 774 (1995).

9. **J. E. Klepeis** and W. A. Harrison, *Charge-state-dependent atomic geometries for isolated metal adatoms on GaAs(110)*, Phys. Rev. B **40**, 5810 (1989).

Refereed–Conference Proceedings

1. A. Landa, **J. Klepeis**, P. Söderlind, I. Naumov, O. Velikokhatnyi, L. Vitos, and A. Ruban, *Ab initio calculations of elastic constants of the bcc V–Nb system at high pressures*, J. Phys. Chem. Solids **67**, 2056 (2006).

2. **J. E. Klepeis**, *Introduction to first-principles electronic structure methods: Application to actinide materials*, in Mat. Res. Soc. Symp. Proc. Vol. 893, edited by J. L. Sarrao, A. J. Schwartz, M. R. Antonio, P. C. Burns, R. G. Haire, and H. Nitsche (Materials Research Society, Warrendale, PA, 2006), p. 3.

3. N. Franco, **J. E. Klepeis**, C. Bostedt, T. Van Buuren, C. Heske, O. Pankratov, and L. J. Terminello, *Valence band study of the PtSi by synchrotron radiation photoelectron spectroscopy*, J. Elec. Spect. Rel. Phenom. **114–116**, 1191 (2001).

4. A. F. Bello, T. van Buuren, **J. E. Klepeis**, and T. W. Barbee, Jr., *Interfacial electronic charge transfer and density of states in short period Cu/Cr multilayers*, in Applications of Synchrotron Radiation Techniques to Materials Science IV, edited by S. M. Mini, S. R. Stock, D. L. Perry, and L. J. Terminello (Materials Research Society, Warrendale, PA, 1998) p. 285.

5. A. F. Bello, T. van Buuren, **J. E. Klepeis**, and T. W. Barbee, Jr., *Electronic effects at interfaces in Cu (Cr, Mo, W, Ta, Re) multilayers*, in Applications of Synchrotron Radiation Techniques to Materials Science IV, edited by S. M. Mini, S. R. Stock, D. L. Perry, and L. J. Terminello (Materials Research Society, Warrendale, PA, 1998) p. 279.

6. A. K. McMahan and **J. E. Klepeis**, *Ab initio calculation of tight-binding parameters*, in Mat. Res. Soc. Symp. Proc. Vol. 491, edited by P. E. A. Turchi, A. Gonis, and L. Colombo (Materials Research Society, Warrendale, PA, 1998), p. 199.

7. **J. E. Klepeis**, C. Mailhiot, M. van Schilfgaarde, and M. Methfessel, *Role of ionicity in the determination of surface atomic geometries: GaP, ZnS, and CuCl (110) surfaces*, J. Vac. Sci. Technol. B **11**, 1463 (1993).

8. **J. E. Klepeis** and W. A. Harrison, *Coverage dependence of Schottky barrier formation*, J. Vac. Sci. Technol. B **7**, 964 (1989).

9. **J. E. Klepeis** and W. A. Harrison, *Electronic structure of small coverages of column III metals on silicon (100)*, J. Vac. Sci. Technol. B **6**, 1315 (1988).

10. **J. E. Klepeis** and W. A. Harrison, *Core electron binding energy shifts and screening in tetrahedral semiconductors*, J. Vac. Sci. Technol. B **5**, 1250 (1987).

Submitted

1. J. R. I. Lee, R. W. Meulenberg, K. M. Hanif, **J. E. Klepeis**, L. J. Terminello, and T. van Buuren, *Experimental observation of quantum confinement in the conduction band of CdSe quantum dots*, Phys. Rev. Lett. (in press).

2. B. Lee, R. E. Rudd, **J. E. Klepeis**, P. Söderlind, and A. Landa, *Theoretical confirmation of a high-pressure rhombohedral phase in vanadium metal*, Phys. Rev. Lett. (submitted).

Non-refereed

1. D. B. Boercker, **J. E. Klepeis**, and C. J. Wu, *Toward improved understanding of material surfaces and interfaces*, Energy and Technology Review, p. 25, August–September, 1994.

2. **J. E. Klepeis**, E. L. Shirley, and M. P. Surh, *Predicting the structural and electronic properties of scintillators*, Energy and Technology Review, p. 33, August–September, 1994.

Ph.D. Thesis

J. E. Klepeis, *Self-consistent electronic structure of semiconductor systems*, Unpublished Ph.D. thesis, Stanford University, Stanford, California, 1989.

PRESENTATIONS

Invited Talks–Actinide Materials at High Pressure

1. *Ab initio study of self-irradiated actinide materials*, JOWOG 32 Materials Meeting, Lawrence Livermore National Laboratory, Livermore, California, March 2006.

2. *Introduction to first-principles electronic structure methods: Application to actinide materials*, Materials Research Society Fall Meeting, Boston, Massachusetts, November 2005.

3. *Ab initio equation-of-state calculations in support of lifetime estimates*, Advanced Simulation and Computing (ASC) Principal Investigators Meeting, Lackland Air Force Base, San Antonio, Texas, February 2005.

4. *BlueGene/L calculations in support of stockpile stewardship*, Initial Meeting on Uses of BlueGene/L for Defense Programs Applications, Los Alamos National Laboratory, Los Alamos, New Mexico, December 2004.

5. *Strength modeling in parallel with high-pressure experiments*, JOWOG 32 Materials Meeting, Atomic Weapons Establishment (AWE), Aldermaston, United Kingdom, November 2004.

6. *Phase diagram, equations-of-state, and strength models for high-pressure actinides*, JOWOG 32 Materials Meeting, Los Alamos National Laboratory, Los Alamos, New Mexico, October 2003.

7. *Properties of high-pressure actinides*, JOWOG 32 Materials Meeting, Atomic Weapons Establishment (AWE), Aldermaston, United Kingdom, February 2001.

8. *High-pressure strength modeling for actinides*, JOWOG 32 Materials Meeting, Los Alamos National Laboratory, Los Alamos, New Mexico, June 1999.

9. *High-pressure elastic constants of actinides*, JOWOG 32 Materials Meeting, Lawrence Livermore National Laboratory, Livermore, California, July 1997.

Invited Talks–Electronic Structure

1. *Chemical bonding in α-Pt_2Si and PtSi*, Universität Erlangen-Nürnberg, Erlangen, Germany, June 2000.

2. *Optical absorption and Fermi surface nesting in platinum and iridium silicides*, Universität Erlangen-Nürnberg, Erlangen, Germany, May 1999.

3. *Atomic and electronic structure calculations for silicide materials*, Universität Erlangen-Nürnberg, Erlangen, Germany, February 1998.

4. *Atomic and electronic structure of cubic and orthorhombic PbF_2*, Xerox Palo Alto Research Center, Palo Alto, California, January 1995.

Invited Talks–Surfaces and Interfaces

1. *Schottky barrier formation for metals on GaAs (110)*, West Virginia University, Department of Physics Colloquium, Morgantown, West Virginia, March 1992.

2. *Metal adatoms on GaAs (110): A Mott-insulator system*, at the Total Energy and Force Methods Workshop, Schloss Ringberg, Tegernsee, Germany, January 1992.

3. *Schottky barrier formation: From isolated adatoms to a fully metallic overlayer*, University of California at Davis, Department of Physics Colloquium, Davis, California, March 1991.

4. *Coverage dependence of Schottky barrier formation*, Lawrence Livermore National Laboratory, Livermore, California, November 1988.

Invited Briefings to External Reviewers–Actinide and other Metals at High Pressure

1. *New directions in EOS and materials theory*, H-Division Technical Review Committee, Lawrence Livermore National Laboratory, Livermore, California, February 2007.

2. *Multiscale strength modeling for bcc Ta: Electronic and atomistic length scales*, Chemistry and Materials Science Directorate Review Committee, Lawrence Livermore National Laboratory, Livermore, California, May 2006.

3. *Aging: From fundamental science to predictive lifetimes*, Enhanced Surveillance Campaign 2006 Annual Review, Lawrence Livermore National Laboratory, Livermore, California, April 2006.

4. *Equation-of-state calculations in support of lifetime estimates*, Advanced Simulation and Computing (ASC) Predictive Science Panel, Los Alamos National Laboratory, Los Alamos, New Mexico, October 2005.

5. *Quantum-based studies of equation-of-state, melt, and phase transition kinetics*, Defense and Nuclear Technologies Directorate Review Committee, Lawrence Livermore National Laboratory, Livermore, California, May 2005.

6. *Improvements to high-pressure strength models*, Advanced Simulation and Computing (ASC) Predictive Science Panel, Lawrence Livermore National Laboratory, Livermore, California, April 2005.

7. *Ab initio equation-of-state calculations for self-irradiated actinide materials*, JASON 2005 Winter Study, General Atomics, San Diego, California, January 2005.

8. *Ab initio equation-of-state calculations on BlueGene/L*, Physics and Advanced Technologies Directorate Review Committee, Lawrence Livermore National Laboratory, Livermore, California, December 2004.

9. *Ab initio equation-of-state calculations for self-irradiated actinide materials*, Lifetime Working Group, Lawrence Livermore National Laboratory, Livermore, California, October 2004.

10. *Calculations for self-irradiated actinide materials and National Ignition Facility (NIF) strength experiments*, H-Division Technical Review Committee, Lawrence Livermore National Laboratory, Livermore, California, April 2004.

11. *Phase diagram, equations-of-state, and strength models for high-pressure actinides*, H-Division Technical Review Committee, Lawrence Livermore National Laboratory, Livermore, California, April 2003.

Contributed Talks–High-Pressure Physics

1. *Fermi surface topology and elastic anomalies in bcc metals at high pressure*, American Physical Society March Meeting, Los Angeles, California, March 2005.
2. *Mechanical instability in bcc vanadium and niobium at high pressures*, American Physical Society March Meeting, Montreal, Canada, March 2004.
3. *Electronic structure of ordered hydrogen/helium alloys at megabar pressures*, American Physical Society March Meeting, Pittsburgh, Pennsylvania, March 1994.

Contributed Talks–Electronic Structure

1. *Optical absorption in hot metals: aluminum and bismuth*, American Physical Society March Meeting, Austin, Texas, March 2003.
2. *Band mapping of single crystal molybdenum disulfide (poster)*, 8$^{\text{th}}$ International Conference on Electronic Spectroscopy and Structure (ICESS8), Berkeley, California, August 2000.
3. *Bonding in platinum silicides*, American Physical Society March Meeting, Minneapolis, Minnesota, March 2000.
4. *Atomic and electronic structure of cubic and orthorhombic PbF_2*, American Physical Society March Meeting, San Jose, California, March 1995.
5. *First-principles electronic structure calculations for cubic and orthorhombic BaF_2 and PbF_2 (poster)*, Materials Research Society Spring Meeting, San Francisco, California, April 1994.

Contributed Talks–Surfaces and Interfaces

1. *Electronic structure of copper lines on the stepped tungsten (110) surface*, American Physical Society March Meeting, St. Louis, Missouri, March 1996.
2. *Atomic and electronic structure of c(2×2) Cl/Cu (001)*, American Physical Society March Meeting, Seattle, Washington, March 1993.
3. *The role of ionicity in the determination of surface atomic geometries: GaP, ZnS, and CuCl (110)*, 20$^{\text{th}}$ Annual Conference on the Physics and Chemistry of Semiconductor Interfaces (PCSI-20), Williamsburg, Virginia, January 1993.
4. *Mott transition for metal adatoms on GaAs (110)*, American Physical Society March Meeting, Indianapolis, Indiana, March 1992.
5. *Overlayer Metallization: Cs on GaAs (110)*, American Physical Society March Meeting, Cincinnati, Ohio, March 1991.
6. *Schottky barrier formation: From isolated adatoms to a fully metallic overlayer*, 18$^{\text{th}}$ Annual Conference on the Physics and Chemistry of Semiconductor Interfaces (PCSI-18), Long Beach, California, January 1991.

7. *Electronic structure and atomic geometry of low coverages of Au on GaAs (110)*, American Vacuum Society Symposium, Toronto, Canada, October 1990.

8. *Atomic geometry of metal adatoms on GaAs (110)*, American Physical Society March Meeting, Anaheim, California, March 1990.

9. *Charge-state-dependent atomic geometries for isolated metal adatoms on GaAs(110)*, American Physical Society March Meeting, St. Louis, Missouri, March 1989.

10. *Coverage dependence of Schottky barrier formation (talk + poster)*, 16$^{\text{th}}$ Annual Conference on the Physics and Chemistry of Semiconductor Interfaces (PCSI-16), Bozeman, Montana, February 1989.

11. *Electronic structure of small coverages of column III metals on silicon (100) (talk + poster)*, 15$^{\text{th}}$ Annual Conference on the Physics and Chemistry of Semiconductor Interfaces (PCSI-15), Asilomar, California, February 1988.

12. *Core electron binding energy shifts and screening in tetrahedral semiconductors (talk + poster)*, 14$^{\text{th}}$ Annual Conference on the Physics and Chemistry of Semiconductor Interfaces (PCSI-14), Salt Lake City, Utah, January 1987.