

DONALD R. HAMANN

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EDUCATION

1957-65 **Massachusetts Institute of Technology**, Cambridge, MA

- **BS** in Electrical Engineering, June 1961.
- **PhD** in Electrical Engineering, June 1965.
- Advisors: Dr. A. W. Overhauser and Prof. G. W. Pratt.
- Dissertation title: *The Wave Vector Dependent Spin Susceptibility of an Interacting Electron Gas.*

EMPLOYMENT

2001 ó **Mat-Sim Research**, Murray Hill, NJ

- President

2001 ó **Rutgers University**, Piscataway, NJ

- Visiting Scientist, Department of Physics and Astronomy.

1965 ó 2001 **Bell Laboratories**, Murray Hill, NJ

- Most recently, Director, Theoretical Materials Physics Research.

EXPERIENCE: Physics Research

1965 ó 70 **Dilute magnetic alloys.**

- Unified inconsistent predictions of properties in the vicinity of the Kondo temperature.[8,9]
- Derived the Fermi-liquid low-temperature limiting behavior of the Kondo effect.[13-15]

1970 ó 80 **Semiconductor surface electronic structure.**

- Introduced realistic calculations of surface states of semiconductors, permitting the interpretation of newly developing ultraviolet photoemission spectroscopies.[20,24]
- Proceeded to study surface reconstruction, adsorbates, and interfaces.[25-49,52-55]

1979 ó 89 **Norm-conserving pseudopotentials.**

- Introduced the principle of norm-conservation for *ab initio* pseudopotentials which allowed accurate calculations of structural phase transitions, vibrational spectra, and many other properties of semiconductors, metals, and insulators.[63,79]
- Generalized this principle to pseudopotentials constructed from scattering wave functions adding flexibility and consistent reference states.[140]

- 1978 ó 85 **Transition metal surfaces and interfaces.**
- Introduced the full-potential linear augmented plane wave method.[59,93]
 - Applied this and the LCAO method to surface states, adsorbates, surface relaxation, and adsorbate vibrational properties.[56,58,61,64,65,67,68,71-73,77,78,83-86, í]
 - Found the structure and electron transmission properties of silicon-silicide interfaces.[126,139]
- 1984 ó 85 **Scanning tunneling microscopy.**
- Derived the quantitative formula relating scanning tunneling microscope images to surface electronic structure, including a theory of STM resolution.[92]
 - Predicted the bias dependence of STM images for semiconductor surfaces.[98,103]
- 1990 ó 93 **Auxiliary-field quantum Monte Carlo methods**
- Derived a diffusive model for the Fermion sign problem.[148]
 - Introduced a new variational approximation for suppressing the sign problem.[146,157]
- 1995 ó 2001 **Properties of SiO₂**
- Demonstrated the critical importance of generalized-gradient corrections in density functional theories of structural energies.[160]
 - Introduced a new mechanism for oxygen diffusion.[167]
 - Developed a model to account for the Si oxidation state in interface simulations.[170]
- 2002 ó 2005 **Density functional perturbation theory.**
- Developed a formalism to treat strain on the same footing as simple perturbations.[176,177]
 - Permits direct calculation of elastic and piezoelectric tensors for solids
 - Derived an analytic theory for strain-induced atomic-relaxation contributions.[179]
- 2002 ó 2005 **Artificially structured oxide superlattices**
- Identified lattice polarization as a key determinant of mobile electron distribution and developed an approximate treatment of finite-temperature anharmonic effects.[180]
- 2007 ó 2009 **Wannier functions for GW quasiparticles**
- Derived formalism for representing quasi-particle-self-consistent wave functions as Wannier functions [181]
 - Allows visualization of GW many-bodyeffects on bonding
 - Facilitates high-resolution GW band-structure analysis
- 2011 ó present **Optimized multi-projector norm-conserving pseudopotentials**
- Combines generalized norm conservation and systematic convergence optimization [183]
 - Achieves the accuracy and efficiency of modern augmented electronic-structure formalisms
 - Permits simple plane-wave basis functions and the ensuing algorithmic and coding simplicity especially important for advanced calculations (eg. DFPT, GW, BSE)
 - Multiple shells of core electrons can be active for extreme-conditions simulations
 - Advanced formulation adds full compatibility with meta-gga density functionals

EXPERIENCE: Computation

- 1969 ó 72 **Laue representation code**
- Developed stable algorithms for numerical integration of the Schrödinger equation in the mixed plane wave-coordinate representation.[20]
 - Employed in full self-consistent program for semi-infinite surface electronic structure calculation.[22,24]
- 1978 **LCAO code**
- Developed Gaussian linear-combination-of-atomic-orbitals density-functional program for bulk solids and slab surface models.[56,58,61,75,76]
- 1979 **FLAPW code**
- Carried out mathematical analysis and algorithm development to extend Andersen's recently introduced linear augmented plane wave electronic structure method from muffin tin to completely general potentials.
 - Developed full-featured program for self-consistent density functional calculations of solids and surfaces.[59,93]
- 1989 **Generalized norm-conserving pseudopotential code**
- Mathematical analysis, algorithms and code for scalar-relativistic electronic structure of all-electron atoms and the generation of these pseudopotentials in semi-local and separable form.[140]
 - Program offered for public distribution, ~100 copies requested.
- 1990 **Quantum Monte Carlo code**
- Analysis, algorithms, and code to explore fermion sign problem for auxiliary-field QMC calculations and new variational approximation.[146-148]
- 1995 ó 2000 **Adaptive Curvilinear Coordinate code**
- Analysis, algorithms, and code for full-featured quantum molecular dynamics program using plane wave basis in adaptive coordinates to enhance convergence with basis size.[158]
 - Novel algorithm to enhance convergence using generalized gradient approximation density functionals.[161].
- 2002 ó present **ABINIT**
- Developer for ABINIT open-source electronic structure project (Advisory Board Member).
 - Added strain perturbation to response function capabilities.
 - Created tutorial on elastic and piezoelectric properties.
 - Added numerous tweaks and bug-fixes.
 - Added GW Wannier function capabilities [181]
- 2013 ó present **ONCVSP open-source pseudopotential code**
- Implements optimized multi-projector norm-conserving potentials [183]
 - Successive releases have incorporated new capabilities
 - A number of users have contributed code for these
 - Used by two groups to produce pseudopotential periodic tables with excellent benchmark performance

Competencies

- Fortran, C, MPI, Mathematica, Unix/Linux system and network management, GIT version control, Myrinet, MS Windows, MS Office.

EXPERIENCE: Research Management

- 1979 ó 81 **Theoretical Physics Research Department**
- Supported 15-20 Members of Technical Staff, postdoctoral fellows, and visiting consultants.
 - Supervised recruiting program for theorists, 1-2 postdoctoral and 0-1 MTS hired annually.
 - Performance review for Physical Research Laboratory, 100 ó 120 professional and support staff.
- 1981 ó 97 **Surface Physics Research Department**
- ÉSupported 10-15 staff members.
 - ÉOversaw development of several major new experimental facilities including 3 beam lines at the National Synchrotron Light Source, an inelastic He beam scattering system at Murray Hill, and an electron energy loss spectroscopy system at MH.
 - ÉPerformance review for Laboratory.
- 1997 ó 2000 **Theoretical Physics Research Department**
- As above, supported 10-15 staff.
- 2000 ó 2001 **Theoretical Materials Research Department**
- Consulting position, no reports.
 - Performance review and policy meetings for Laboratory.

RECOGNITION

- 1972 **Fellow** of the American Physical Society.
- 1979 **Davison-Germer Prize** of the American Physical Society
- Citation: *For his pioneering analyses of the electronic structure of semiconductor surfaces.*
- 2001 **ISI Most Cited Researcher**
- Physics category.
- 2001 **Cosslett Award** of the Microbeam Analysis Society
- Citation: *“Current Limits in Predicting EELS fine Structure.”*

PROFESSIONAL SERVICE

- 2000 ó 2005 **American Institute of Physics**
ÉGoverning Board member, 2000 ó 2003.
• Nominating Committee, 2001.
• State Department Science Fellowship Selection Committee, 2001 ó 2004; chair 2004.
• Committee on Committees, 2003-2005.
- 1984 ó 2003 **American Physical Society**
ÉExecutive Board member, 1998 ó 2000.
• Council, general councilor, 1996 ó 2000.
• Membership Committee, 2000 ó 2003 .
• Task Force to Review Physical Review B, 1999 ó 2000.
• Task Force on the Structure of the Council, 1998 ó 1999.
• Division of Condensed Matter Physics Executive Committee member, 1984 ó 89.
- 1981 ó 87 **International Union of Pure and Applied Physics**
• Semiconductor Commission, US representative.
- 1980 ó 92 **Physical Electronics Conference**
• General Committee Chairman, 1989 ó 92.
• General Committee member, 1980 ó 82.

REFERENCES

Available upon request

**D. R. HAMANN
PUBLICATION LIST**

1. **A Matched Amplifier Using Two Cascaded Esaki Diodes**, D. R. Hamann, *Proc. IRE* **49**, 904 (1961).
2. **Cascade Capture of Electrons by Ionized Impurities**, D. R. Hamann and A. L. McWhorter, *Phys. Rev.* **134**, A250 (1964).
3. **Electron-Gas Spin Susceptibility**, D. R. Hamann and A. W. Overhauser, *Phys. Rev.* **143**, 183 (1966).
4. **The Effective Mass of Positrons in Metals**, D. R. Hamann, *Phys. Rev.* **146**, 277 (1966).
5. **Self-Consistent Curie-Law Calculation for Anderson's Dilute-Alloy Model**, D. R. Hamann, *Phys. Rev. Lett.* **17**, 145 (1966).
6. **Properties of Magnetically Dilute Alloys**, D. R. Hamann and T. H. Geballe, *Magnetism and Magnetic Materials: 1966 Digest*, ed. by C. W. Haas and H. S. Jarrett (Academic, New York, 1966), p. 71.
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17. **Investigation of Kondo Alloys and Compound by the Superconductive Proximity Effect**, J. J. Hauser, D. R. Hamann, and G. W. Kammlott, *Phys. Rev. B* **3**, 2211 (1971).
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19. **Variational Calculation of the Image Potential Near a Metal Surface**, J. A. Appelbaum and D. R. Hamann, *Phys. Rev. B* **6**, 1122 (1972).
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21. **Functional Integral Methods in the Magnetic Impurity Problem**, D. R. Hamann and J. R. Schrieffer, in *Magnetism*, Vol. V, ed. G. T. Rado and H. Suhl (Academic, New York, 1973) p. 237.
22. **Self-Consistent Pseudopotential for Si**, J. A. Appelbaum and D. R. Hamann, *Phys. Rev. B* **8**, 1777 (1973).
23. **X-Ray Photoelectron Spectroscopy of Implanted Rare Gasses in Nobel Metals: Polarization and Potential Effects**, D. R. Hamann and P. H. Citrin, *Chem. Phys. Lett.* **22**, 301 (1973).
24. **Surface States and Surface Bonds of Si(111)**, J. A. Appelbaum and D. R. Hamann, *Phys. Rev. Lett.* **31**, 106 (1973).
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26. **Measurement and Calculation of Polarization and Potential-Energy Effects on Core-Electron Binding Energies in Solids: X-Ray Photoemission of Rare Gases Implanted in Noble Metals**, P. H. Citrin and D. R. Hamann, *Phys. Rev. B* **10**, 4948 (1974).
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