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 – **Mat-Sim Research**, Murray Hill, NJ
• President

2001 – **Rutgers University**, Piscataway, NJ
• Visiting Scientist, Department of Physics and Astronomy.

1965 – 2001 **Bell Laboratories**, Murray Hill, NJ
• Most recently, Director, Theoretical Materials Physics Research.

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EXPERIENCE: Physics Research

1965 – 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 – 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 – 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 – 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, …]
• Found the structure and electron transmission properties of silicon-silicide interfaces.[126,139]

1984 – 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 – 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 – 2001 **Properties of SiO_2**
• 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 – 2005 **Density functional perturbation theory.**
• Developed a formalism to treat strain on the same footing as simple perturbations.[176]
• Derived an analytic theory for strain-induced atomic-relaxation contributions.[178]

2002 – 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.[179]

EXPERIENCE: Computation

1969 – 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 – 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]
• Parallel version developed which yields excellent scaling on Beowulf-class computers.

2002 – 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.

Competencies
• Fortran, C, MPI, Mathematica, Unix/Linux system and network management, Myrinet, MS Windows, MS Office.

EXPERIENCE: Research Management

1979 – 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 – 120 professional and support staff.

1981 – 97 **Surface Physics Research Department**
• Supported 10-15 staff members.
• Oversaw 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.
• Performance review for Laboratory.

1997 – 2000 **Theoretical Physics Research Department**
• As above, supported 10-15 staff.

2000 – 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 – 2005 **American Institute of Physics**
• Governing Board member, 2000 – 2003.
• Nominating Committee, 2001.
• State Department Science Fellowship Selection Committee, 2001 – 2004; chair 2004.
• Committee on Committees, 2003-2005.

1984 – 2003 **American Physical Society**
• Executive Board member, 1998 – 2000.
• Council, general councilor, 1996 – 2000.
• Membership Committee, 2000 – 2003 .
• Task Force to Review Physical Review B, 1999 – 2000.
• Task Force on the Structure of the Council, 1998 – 1999.
• Division of Condensed Matter Physics Executive Committee member, 1984 – 89.

1981 – 87 **International Union of Pure and Applied Physics**
• Semiconductor Commission, US representative.

1980 – 92 **Physical Electronics Conference**
• General Committee Chairman, 1989 – 92.
• General Committee member, 1980 – 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**, l83 (1966).

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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).

20. **Self-Consistent Electronic Structure of Solid Surfaces**, J. A. Appelbaum and D. R. Hamann, *Phys. Rev. B* **6**, 2166 (1972).

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.

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31. **Self-Consistent Quantum Theory of Chemisorption: H on Si(111)**, J. A. Appelbaum and D. R. Hamann, *Phys. Rev. Lett.* **34**, 806 (1975).

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