

Biography of J. Woods Halley

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Personal:

born November 16, 1938, Chicago, IL

married to Merile Hobbs (d. 2001), 2 children.

Education:

B.S., M. I. T., 1961

Ph.D., University of California, Berkeley, 1965 (Thesis Advisor, C. Kittel)

Positions:

Teaching Assistant, University of California, Berkeley, 1961 - 63

NSF Predoctoral Fellow, University of California, Berkeley, 1963 - 65

NSF Postdoctoral Fellow, Faculte des Sciences, Orsay, France, 1965 - 66

Assistant Professor, University of California, Berkeley, 1966 - 68

Associate Professor, University of Minnesota, Minneapolis, 1968 - 77

Professor of physics, University of Minnesota, 1977 - present

Fellow of the Supercomputer Institute, University of Minnesota, 1989-present

Graduate Faculty of Materials Science, University of Minnesota, 1989- 2012

Visiting positions at Oxford Univ.(1973),Harwell AERE (1973),Univ. of Oregon (1975), Yale (1976), Brookhaven (1976, 1979), Harvard (1979), Michigan State (1980), Argonne (1981-1993) ,Institute for Theoretical Physics, Santa Barbara (1983), University of California, Santa Barbara, Chemistry Department (1984), IBM Almaden Research Center (1987), Australian National University(1988), University of California, Berkeley, Chemistry Department (1993), Institute for Theoretical Physics, Santa Barbara (1997, 1998).

Societies:

APS, AAAS, MRS, ACS

Honors:

NSF Predoctoral Fellow, 1963 - 65

NSF Postdoctoral Fellow, 1965 - 66

George Taylor Teaching Award 1979

McMillan Professorship, 1979

Bush Fellowship, 1983-84

IBM Paul J. Flory Sabbatical, 1987

Fellow of the American Physical Society, 1998-present

NSF Grants 1972 - 79; Research Corp. Grant 1970 - 72; Corrosion Center Grant 1980 - 92; Educational Development Program grants 1973, 1979; Quarter leaves 1973, 1979, 1988, 1993; U. of Minn. Summer Research grants 1969, 1982; 3M grant 1982, IBM Advanced Education Project Grant, 1985; Dept. of Education grant, 1986, NSF US-Australia travel grant, 1987; IBM Sponsored University Research Grant 1988-90; Electric Power Research Institute grant, 1988-90; Dept. of Energy grant, Materials Sciences 1991-2005; Sumitomo Metal Industries grant 1992-93; National Aeronautics and Space Administration grant 1992-95; DOE grant, Basic Energy Sciences (batteries) 1993-2006; NSF grants: Condensed Matter Theory 1995-98, Condensed Matter Experiment 1999-2001, International Division 1999-2008; 3M DOE subcontract, 2003-2005, Argonne subcontract 2005-2008, CURA internal University of Minnesota grant 2008-2011.

Current research interests: Simulation methods for description of materials properties and properties on intermediate scales, based on first principles data. A method for renormalising molecular dynamics models for use on coarser scales is being developed. Development continues on our suite of first principles based tight binding codes, currently used by groups at Argonne, in Florida and in Pittsburg (NETL, DOE Lab). The tight binding codes are being applied to studies of oxygen reduction on platinum and to water dissolution on titania. A small experimental group studies alternative materials for water electrolysis. We continue to carry out experiments on transmission of atomic beams through films of superfluid helium with supporting many body computational studies. A statistical mechanical model of the origin of life is studied.

Professional Activities:

National Research Council Panel on NSF Predoctoral Fellowships, 1976, Chairman 1977, 1978

NATO Advanced Study Institute, Director and Proceedings Editor, 1977

Conference on Magnetism and Magnetic Materials, 1977; session chairman, registration committee.

Midwest Theory Conference, session chairman 1978, 1981; committee chairman and proceedings editor, 1984.

Contributor to National Materials Advisory Board report on Electrochemical Corrosion, 1985

DOE Panel on Fuel Cells and Batteries, 1987

Minnesota Theoretical Physics Institute Workshop on Mechanisms of High Temperature Superconductivity, Director, 1987.

US Committee for Scientific Cooperation with Vietnam, Physics board member, 1985-present.

Consultant: 3M, 1985-1989; UNESCO, 1986; General Motors Corp, 1989-90; Educational Testing Service, 1989; National Renewable Energy Laboratory, 1994-95; Pacific Northwest Laboratory 1995.

International Symposium on High T_c Superconductivity, Hanoi, 1990, member of the organizing committee.

Committee of Examiners for the Graduate Record Examination in Physics, Educational Testing Service, 1990-1996.

Electrochemistry Society Symposium on Microscopic Models of the Electrode-Electrolyte Interface and Corrosion Processes, Toronto, 1992 co-chair.

Seventh International Conference on Progress in Many Body Theories, Minneapolis, 1991, member of the organizing committee.

Introductory University Physics Project (NSF, AIP), evaluation test site investigator, 1991-92.

Conference on the Role of the Condensate and Vorticity in Dense Bose Systems, Minneapolis, 1993 (LT20 Satellite). Director and proceedings editor.

DOE Corrosion Contractors' meeting, Minneapolis, 1997,organiser.

Symposium on Theory of Electrochemical Interfaces, American Chemical Society meeting, New Orleans, 1999, organiser; proceedings editor.

Symposium on Global Climate Change and the Chemical Industry: Renewable technologies and new frontiers , American Institute of Chemical Engineers New Orleans, 2002, session organiser and chair.

Basic Energy Sciences Advisor Committee Workshop on Future of Energy Research, Department of Energy, Gaithersburg, MD, 2003

Workshop on Hydrogen Economy, Department of Energy, Rockville, MD, 2003

Workshop on Yucca Mountain Nuclear Waste Depository, Department of Energy, Bethesda, MD, 2003

NSF MRSEC Review Panel, Northwestern University, 2003

DOE Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program national review panel, 2012,2014,2015.

Advisory board for Energy Frontier Research Center, the Center for Electrochemical Energy Science (CEES), Argonne National Laboratory, 2014-2016

References:

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Research Accomplishments of J. W. Halley:

Current Research Interests:

Theory of disorder in condensed matter, statistics and dynamics of polymers, physics of the fluid-solid interface, high temperature superconductivity, condensate fraction in bose superfluids.

(Footnotes refer to papers in publication list.)

Theory of Second Order Optical Spectroscopy

Identified the first two spin wave optical process³⁻⁷ (in collaboration with I. Silvera). Predicted two roton Raman scattering in liquid helium¹⁰⁻¹². Later work has refined the early work in this field by: 1) studies of microscopic mechanisms in magnets^{13,14,18}; 2) study of two spin wave processes in one dimensional paramagnets^{23,32,48}; 3) establishing connections between two-roton scattering and uv absorption^{15,27,82,101,122}; and 4) studies of side bands of impurity absorption in classical liquids^{17,22}. Identified light scattering technique for study of energy fluctuation in magnets.⁴⁷

Theory of Liquid Helium

Accounted theoretically for the "neutral current" discovered by Surko and Reif.^{19,28} Proposed experiments to measure vortex and bubble oscillations.^{9,24,35} Removed long-standing objection to the pairing approximation in the interacting boson problem.^{26,30,36} Established rigorous limits on the usefulness of the quasi-particle approximation for liquid helium.^{25,31} Identified new contributions to superfluid density.⁵⁵ Proposed new experiment to observe condensate fraction^{67,123,124,125,126,145,158,162,186}. Demonstrated new method for suspension of a superfluid slab and used it to measure cesium-helium contact angle¹³⁸.

Theory of Dynamics of One and Two Dimensional Magnetic Materials

Introduced Green function decoupling scheme for paramagnets²⁰ which was later widely applied to 1d materials. Application to the dimerized chain raised basic questions concerning the nature of the spectrum³³. Studied various approximations schemes^{34,37}.

Theory of Disordered Materials

Calculated zero point effects in dilute antiferromagnetic nets^{42,43}. Formulated chemically constrained polychromatic percolation model and applied to metal insulator problem.^{45,49} First correctly defined and estimated dimension of the large percolation cluster.⁵⁰ Defined and studied AB percolation and related models.^{52,57} Found phase diagram for a spin glass model with finite and infinite range interactions.⁵⁴ Analysed Almeida-Thouless instability in experiment with ferromagnetic couplings⁶⁰ Studied coulomb glass on percolation clusters.⁶⁶, new numerical methods in the localisation problem^{79,93,102,109,114}. Model for role of disorder in high T_c superconductors^{81,97,98,112,115}. Developed models of disordered oxides^{105,116,121,130,133,149}

Theory of Electrolytes and the Electrolyte-Solid Interface

Established relations of molten salt dynamics to the dynamics of the solid.⁴⁶ Developed new double layer theory for metal-electrolyte interface.^{59,68,72,77,85,119,134,136,143,144,146,147,151}

Made electron transfer calculations for the metal-electrolyte interface.^{58,88,103,128,141} Made molecular dynamics studies of statics^{73,91} and dynamics⁷⁴ of multivalent cations in aqueous solution. Introduced new methods in the treatment of molecular polarizability in molecular dynamics of molten salts⁸⁴. Made new self-consistent theory of tunneling across interfaces⁷⁶. New methods for treating Coulomb interactions in molecular dynamics simulations of a fluid at an interface^{89,90,142}. Dissociable molecular dynamics model of water¹¹⁷. Studies of Jahn Teller effect in liquids^{113,118,131}. Demonstrated use of magnetite in hydrogen generating water electrolyzers¹⁸⁹. Studies of CO₂ adsorbing solids^{190,192}

Theory of Polymer Dynamics and Structure

Identified two phonon lines in Raman spectrum of polyethylene³⁸ and studied final state interactions between the phonons⁴⁰. Studied harmonic dynamics of a disordered zig-zag chain,^{61,69} statistics of biased self-avoiding walks^{64,75,78} and Levy flight.⁶⁵ Formulated new theory of the rod-to-coil transition⁷⁰, and of phases of amphiphiles and water⁸⁰. New study of finite size effects in polymers⁸³. Predicted chemical behavior of water in glassy polymers^{92,96} and anomalous diffusive behavior in the same problem⁹⁵. Produced model of amorphous regions of polymer electrolytes^{139,150} and used it to study ion transport¹⁴⁰ and ion pairing¹⁵⁵ in those electrolytes. Introduced renormalization methods for extension of temporal range of polymer simulations[157]. Studies of mechanism of lithium transport in battery electrolytes[163] was featured in a Department of Energy "high light" in 2000. Elucidated mechanisms of proton transport in ionic liquids¹⁸⁴

A selection of five most significant papers of J. W. Halley.

In selecting these I opted for papers of which the significance is already widely, if not universally, recognised. This criterion left out things in the literature which I think might still prove to be of long term significance, such as our papers on an experiment to observe the condensate fraction and a model for point defect induced superconductivity.

1."Infrared Absorption in FeF₂ Phenomenological Theory" (with I. Silvera) Phys. Rev. 149, 415 (1966). This ancient paper identified the first two magnon optical process and set off a large amount of activity in which a great many such processes were identified and studied, sometimes in existing data where they had not been recognised. The processes were later used to study magnon interactions. Similar experiments in recent years have been used to sort out magnetic properties of high temperature superconductors and some of my 30 year old papers were used and cited in that effort.

2."Theory of Optical Processes in Liquid Helium" pp. 175-184 of Proceedings of the Int'l conf. on Light Scattering Spectroscopy edited by George Wright, Springer-Verlag, Inc., New York (1968). This paper (and a related one in Physical Review about the same time) motivated Tom Greytak to do the experiments which led to the discovery of the two roton optical process. Many people, including my group with NSF support, worked on understanding various aspects of this during the 1970's. In the 1980's a Japanese group in Hiroshima experimentally confirmed some of our predictions concerning the ratio of d wave to s wave components in the scattering. The theoretical understanding of this process is incomplete. Some of the theoretical work by other on bound states in the 1970's was based on incorrect physical assumptions, as demonstrated by my post doc, Peter Kleban in 1974. In the last 10 years I have collaborated with Michael Korth in an effort to improve the theoretical description. I reviewed the situation in an invited talk at a satellite conference at the Low Temperature conference in Sussex in 1990.

3. "Numerical Estimates of the Hausdorff Dimension of the Largest Cluster and Its Backbone in the Percolation Problem in Two Dimensions"(with Thang Mai), Phys. Rev. Lett. 43, 740 (1979). Though its numerical results were later superceded, this

paper was widely acknowledged to be the first to state the right definition (consistent with Hausdorff) of the fractal dimension of the large cluster in percolation. It is referenced in the second edition of Mandelbrot's book. Our later work in percolation was mainly on extensions of the model, including AB percolation, which has stimulated a great deal of activity in the applied mathematics community. Our work on these models was summarized in an invited review published in a book called "Percolation Structures and Processes" edited by Adler, Deutcher and Zallen, which appeared in 1983. There has recently been some revival of interest in such models, represented by papers in Physical Review Letters.

4."A New Model of the Differential Capacitance of the Double Layer" (with D. Price), *J. Electroanal. Chem.* 150, 347(1983). This paper was the first in a long series which we have published on the effects of conduction electrons on the electrostatic properties of the metal water interface. The paper introduced two ideas which were strange to the physical electrochemistry community: 1) that the conduction electrons do indeed contribute significantly to the observed macroscopic electrostatic properties (such as differential capacitance) and 2) that significant amounts of displacement of the solvent molecules near the interface occurs as a result of the response of the conduction electrons to changes in the interfacial potential drop. Several other workers (but not all electrochemists!) recognised 1) at about the same time, but I do not think that any of them had 2) right at first.

5."Simulation Study of the ferrous-ferric electron transfer at a metal- aqueous electrolyte interface" with B. Smith, *J. Chem. Phys.* 101, 10915(1994). I believe that this work with Barton Smith has significantly changed the paradigm for study of electron transfer reactions at metal solvent interfaces. The numbers look good but more significantly, the topology of the relevant free energy surface (including the space in which it is to be represented!) were significantly clarified in my opinion. Sociological evidence for this includes widespread imitation and citation. Recent invitations to contribute to special journal issues and a book as well as to organise a symposium at the American Chemical Society meeting in 1999 are evidence of the growing impact of this line of our work. One can also mention the improvements on this calculations introduced by Sean Walbran in his thesis on the cuprous-cupric electron transfer.

Publications of J. W. Halley:

Edited books:

1. **Correlation Functions and Quasiparticle Interactions**, Plenum Press, N.Y., 1978 (Proceedings of a NATO Advanced Study Institute held in Minneapolis in 1977)kip-6pt
2. **Surfaces and Disorder** Materials Science Forum, volume 4 Trans Tech Publications, Aedermannsdorf, Switzerland(1985)
3. **Theories of High Temperature Superconductivity** Addison-Wesley, Reading, MA, 1988
4. **Models of the Electrode-Electrolyte Interface** (with L. Blum)Proceedings Volume 93-5 of the Electrochemistry Society(1993).
5. **The Role of the Condensate and Vorticity in Dense Bose Systems** , December 1993 issue of Journal of Low Temperature Physics.
6. **Solid Liquid Interface: Theory** ,American Chemical Society Publications (2001)

Published books:

Physics of Human Motion, Burgess, Minneapolis, 1981

Statistical Mechanics Cambridge University Press, 2006

How Likely Is Extraterrestrial Life? Springer-Verlag, 2012

Papers

1. "L Fluorescence Yields in Heavy Elements" (with D. Engelkemeir), Phys. Rev. 134, A24 (1964)
2. "Molecular Binding in the Limit of Very Large Spin-Orbit Interaction" (with H. Shore), J. Chem. Phys. 42, 597 (1965)
3. "Odd-Exciton Magnon Interaction and Anomalous Far-Infrared Absorption in FeF_2 " (with I. Silvera), Phys. Rev. Letters 15, 654 (1965).
4. "Infrared Absorption in FeF_2 Phenomenological Theory" (with I. Silvera) Phys. Rev. 149, 415 (1966).

5. "Microscopic Theory of Far-Infrared Two-Magnon Absorption in Antiferromagnets. I. Perturbation Theory Search and Application of Fourth-Order Process to FeF_2 ", Phys. Rev. 149, 423 (1966).
6. "Microscopic Theory of Far-Infrared Two-Magnon Absorption in Antiferromagnets. II. Second Order Process and Application to MnF_2 ", Phys. Rev. 154, 458 (1967)
7. "Observation and Theory of New Line in Far-Infrared Absorption in Antiferromagnetic FeF_2 " (with I. Silvera), J. Appl. Phys. 37, 1226 (1966).
8. "Theory of Hyperfine Parallel Resonance in Ferromagnets with Application to $K_2CuCl_4 \cdot 2H_2O$ " Phys. Rev. 168, 593(1968)
9. "Theory of Vortex Resonance in Liquid Helium" (with A. Cheung), Phys. Rev. 168, 209 (1968), Erratum, Phys. Rev. A1, 1272 (1970).
10. "Raman Scattering in Liquid Helium" Bull. Amer. Phys. Soc. 13, 398 (1968).
11. "Mechanism for Two-Roton Raman Scattering in Liquid Helium" Phys. Rev. 181, 338 (1969).
12. "Theory of Optical Processes in Liquid Helium" pp. 175-184 of Proceedings of the Int'l conf. on Light Scattering Spectroscopy edited by George Wright, Springer-Verlag, Inc., New York (1968).
13. "Some Possible Experiments for Study of Mechanism of Two Spin-Wave Scattering and Absorption" ibid. pp. 207-220.
14. "Stark Effects in Rutile Antiferromagnets" Journ. of Applied Physics 40, 987 (1969).
15. "Theory of Optical Absorption of a Simple Liquid with Application to Liquid Helium" (with M. Gillan) Phys. Rev. A1, 484 (1970).
16. "Spin-Waves in $He^3 - He^4$ Mixtures" (with Hing-Tat Tan), Physics Letters 35A, 443 (1971).
17. "Collective Effects in the Optical Absorption of Diatomic Molecules in Simple Liquids" (with M. Gillan) Phys. Rev. A4, 684 (1971).
18. "Theory of Infrared Absorption by Cobalt Ion Pairs in MgF_2 " Journ. of Applied Physics 42, 1647 (1971).
19. "Possible Origin of the Neutral Current in Liquid Helium" (with Clayton Giese), Physics Letters 37A, 59 (1971).
20. "Decoupling Scheme for the Heisenberg Ferromagnet above the Transition Temperature" (with S.K. Lo), AIP Conference Proceedings Series 5, 378 (1972).
21. "Temperature Fluctuations Associated with Gravity Waves at a Vapor-Superfluid Interface", Phys. Rev. A5, 1807 (1972). Errata, Phys. Rev. A8, 575 (1973).
22. "Absorption by Dilute Solutions of H_2 in Liquid Argon," (with W. Holcomb), Phys. Rev. A7, 694 (1973).
23. "Fourth Order Green's Function Decoupling for One-Dimensional Antiferromagnets -Application to Optical Properties of TMMC" (with S.K. Lo), Physical Review B8, 5272

(1973).

24. "Possible Resonances in the Mobility of Negative Ions in the Presence of a Microwave Field", Journal of Physics C7, 1462 (1974).

25. "Quantitative Study of the ZRS Model of the Dynamics of Liquid Helium" (with R. Hastings), Phys. Rev. A10 2488 (1974).

26. "Phenomenological Two-Branch Model for the Long-Wave Length Excitation Spectrum of Superfluid He_4 " (with R. Hastings) Phys. Rev. B12, 267 (1975).

27. "Estimate of Integrated Raman Scattering Intensity from the 2^1P_1 Ultra-Violet Absorption Line Shape in Liquid Hel (with P. Kleban), Phys. Rev. B11, 3520 (1975).

28. "Temperature Dependence of the Neutral Current in Liquid Helium," (with W. Holcomb), J. Low Temp. Phys. 20, 365 (1975).

29. "A Course in Physics of Human Motion," (with B. Eaton), Amer. Jour. of Physics 43, 1007 (1975).

30. "Boson Pairing in the RPA," (with R. Hastings), Phys. Rev. B13, 3749 (1976).

31. "Results on the Quasiparticle Model for Liquid He_4 at Finite Temperatures," Phys. Rev. B15, 1404 (1977).

32. "Theory of Two Spin Infrared Absorption in One Dimensional Antiferromagnets, Improved Green Function Theory and Classical Moments," (with M. Drawid), Phys. Rev. 15, 413 (1977).

33. "Spin Dynamics of a Dimerized Heisenberg Chain," (with M. Drawid), A.I.P. Conference Proceedings 34, 208 (1976)

34. "Approximations to the Mori Continued Fraction in Paramagnets," (with M. Drawid) A.I.P. Conference Proceedings 34, 211 (1976).

35. "A New Calculation of the Ion Velocity Shift in a Vortex Resonance Experiment in HeII" (with R. Ostermeier), Journal of Low Temperature Physics 26, 877 (1977).

36. "Exact Solution to the Pairing Equations for Bosons in a One-Dimensional Model" Journal of Low Temperature Physics 26, 129 (1976).

37. "The Truncation of the Mori Continued Fraction for the Spectral Function in Heisenberg and XY models (with M. Drawid), Journal of Phys. and Chem. of Solids, 38, 1269-74 (1977).

38. "Theory of Second Order Raman Scattering from a Zig-Zag Chain with Application to Polyethylene," (with P. Kleban and J. Onffroy), Journal of Polymer Science: Polymer Physics Edition 16, 189-200 (1978).

39. "Electron-Electron Interaction Due to Molecular Modes in a Metal-Ammonia Mixture," Physical Review B18, 4685 (1978).

40. "Final State Interactions in the Two Phonon Raman Spectrum of the Zig-Zag Chain (with J. Onffroy) Journ. Phys. and Chem. of Solids 39, 625 (1978).

41. "Observability of the Beliaev Terms in Inelastic Neutron Scattering from Liquid

- Helium Four," Physical Review, Phys. Rev. B17, 1462 (1978).
42. "Mean Spin per Site in the Linearized Spin Wave Theory of a Dilute Two Dimensional Antiferromagnet," (with W.K. Holcomb), J. Phys. C11, 753 (1978).
43. "Behavior of the Mean Spin on Finite Clusters in a Model for the Dilute Heisenberg Antiferromagnet (with W.K. Holcomb), J. Appl. Phys. 49 (3), 2153 (1978).
44. "Simple Model for Characterizing the Electrical Resistivity of A - 15 Superconductors," (with H. Weisman, M. Gurvitch, H. Lutz, A. Ghosh, B. Schwarz, M. Strongin, and P. Allen), Phys. Rev. Lett. 38, 782 (1977).
45. "Conductivity of a Three Component 'Reactive' Percolation Model (with W. Holcomb), Physical Review Letters 40, 1670 (1978).
46. "Dynamics of Molten Salts", (with M. Feinsein and P. Schofield), Journ. of Physics C12, 4185 (1979).
47. "Light Scattering as a Probe of Dynamical Critical Properties of Antiferromagnets, Phys. Rev. Letters 41, 1605 (1978).
48. "Fluctuations of the Energy-Energy Correlation Function of One- Dimensional Magnetic Models" (with D. Bowman), J. Appl. Phys. 50 (3), 1768 (1979).
49. 'Infinite clusters in quenched *AB* alloys' M. Barma and J.W. Halley, Nucl. Phys. and Solid State Phys. Symposium (India) 22C, 493 (1979).
50. "The Conduction Problem in Multicomponent Percolation" (with W. Holcomb and K. Goetz), Phys. Rev. B21, 4840 (1980).
51. "Numerical Estimates of the Hausdorff Dimension of the Largest Cluster and Its Backbone in the Percolation Problem in Two Di- mensions (with Thang Mai), Phys. Rev. Lett. 43, 740 (1979).
52. "Integrated Polarized Light Scattering from Liquid *He*₄ "(with C. Campbell and F. Pinski), Phys. Rev. B21, 1323 (1980).
53. "AB Percolation on a Triangular Lattice," (with Thang Mai) in Ordering in Two Dimensions, Ed. S. Sinha, North Holland, N.Y., p. 369 (1980).
54. "Scaling in Superconductor-Insulator Mixtures," Solid St. Comm., 40, 19 (1981).
55. "A Spin Glass Model with Short and Long Range Interactions," (with D. Bowman, Phys. Rev. B25, 1892 (1982).
56. "Sum Rule Relating Pair Fluctuations and the Superfluid Mass Density in Helium Four" Physica 108B, 1389-90 (1981).
57. "Scaling Relations and Analytic Solution for the Thomas-Fermi Metal -Dielectric Surface," (with D. Dahl), Journ. Chem. Phys. 77(3), 1611 (1982).
- 58 "Polychromatic Percolation", in **Percolation Structures and Processes** edited by G. Deutscher, R. Zallen, J. Adler, Annals of Israel Physics Society 5, (Adam Hilger, Bristol, 1983) p. 323-352.
59. "Ab Initio Calculation of Electron Transfer Rates in a Model of the Metal-Electrolyte

- Interface," (with S. Pratt and B. Johnson), J. Electroanal. Chem. 150, 355(1983)
60. "A New Model of the Differential Capacitance of the Double Layer" (with D. Price), J. Electroanal. Chem. 150, 347(1983).
61. "High field Magnetization Studies on an Amorphous Alloy with 'Para,' 'Ferro' and 'Spin-glass' regions" (with K.V. Rao, J. Gerber and H.S. Chen), J. Appl. Phys. 53(11), 7731(1982).
62. "Harmonic Modes of a Disordered Zig-Zag Chain" (with M. Thorpe and A. Walker) Journ. of Poly. Sci., Poly. Symp. E 73, 55(1985)
63. " $T_c(p)$ for a Disordered Superconductor" (with K.L. Yao) ,Phys. Rev. B 29, 6207(1984).
64. "Percolation and Related Systems in Equilibrium Statistical Mechanics," (with C. Das Gupta), in **The Mathematics and Physics of Disordered Media**, ed. by B. D. Hughes and B. W. Ninham, Lecture Notes in Mathematics 1035, 260(1984), Springer-Verlag, Berlin.
65. "Scaling in Biased Random Walks (with H. Nakanishi and R. Sunderarajan) ,Phys. Rev. B. 31, 293(1985)
66. "Self Avoiding Levy Flight" (with H. Nakanishi) Phys. Rev. Letters 55, 551(1985)
67. "Nonlinear Response and Metastability of Coulomb Systems Near the Percolation Threshold " (with Y. Gefen) in "Kinetics of Aggregation and Gelation", F. Family and D. P. Landau, eds. ,Elsevier Science Publishers, B. V., Amsterdam (1984) pp 161-164
68. "Proposal for Measurement of order Parameter Statics and Dynamics in Liquid Helium Four",LT-17(Contributed Papers),U. Eckern, A. Schmid, W. Weber,H. Wuhl(eds), Elsevier Science Publishers B. V. (1984) p. 1207
69. "Quantum Theory of the Double Layer: A Model of the Electrode-Electrolyte Interface" (with B. Johnson, D. Price and M. Schwalm), Phys. Rev. B 31, 7695(1985)
70. "Numerical Studies of the Harmonic Modes of a Disordered Zig-Zag Chain" (with J. Onffroy, M.F.Thorpe and A. B. Walker) , Phys. Rev. B32 2132(1985)
71. "Role of Long-Wavelength Degrees of Freedom in the Rod-to-Coil Transition in Polymers" (with N. Goldenfeld), Physical Review Letters 55, 730 (1985)
72. "Numerical Studies on the Renormalization of Mass Matrices" (with E. A. Paschos and H. Usler) , Physics Letters 155B, 107 (1985)
73. "Topics in the Physics of Electrochemistry", Superlattices and Microstructure 2, 165(1986)
74. "Nonadditivity of Ab Initio Pair Potentials For Molecular Dynamics of Multivalent Transition Metal Ions in Water (with L. Curtiss, J. Hautman and A. Rahman), J. Chem. Phys. 86, 2319 (1987)
75. "Molecular Dynamics Study of Raman Scattering and Infrared Absorption of Ferrous and Ferric Ions in Aqueous Solution" (with J. Hautman), Ber. Bunsenges. Phys. Chem. 91, 491 (1987)

76. "Stiff Chains and Levy Flight: Two Self-Avoiding Walk Models and the Uses of Their Statistical Mechanical Representations", in "Percolation Theory and Ergodic Theory of Infinite Particle Systems", H. Kesten, editor, The IMA Volumes in Mathematics and its Applications, vol. 8, p. 169 Springer-Verlag, NY (1987)
77. " Self Consistent Model for Tunneling Across a One-Dimensional Barrier in A Many Electron System" (with D. Dahl), in "Condensed Matter Theories, Vol. 2 " p.149, R. Kalia and P. Vashishta, editors Plenum Press,N.Y.(1987)
78. "Quantum Theory of the Double Layer:Model Including Solvent Structure" (with D.Price), Phys. Rev. B35, 9095 (1987)
79. "A New Spin Model for the Biased Self-Avoiding Walk" (with D.Atkatz, G.ten Brinke and H. Nakanishi, Phys. Rev. B36, 5500 (1987)
80. " Equation of Motion Method for the Study of Defects in Insulators: Application to a Simple Model of TiO_2 ." (With Herbert B. Shore) , Phys. Rev.B36, 6640 (1987)
81. "Model for Bulk Phases in Mixtures of Amphiphilic Molecules and Water" (with A.J.Kolan), J. Chem. Phys. 88,3313 (1988)
82. "Model for the Role of Oxygen Defects in Oxygen Defect Superconductors" (with H.B. Shore), Phys. Rev. B37, 525 (1988)
83. "Theory of Inelastic Light Scattering from 4He ", in "Elementary Excitations in Quantum Fluids", K. Ohbayashi and M. Watabe, eds. Springer-Verlag Series in Solid State Sciences 79, Springer-Verlag, Heidelberg (1989),p. 106 Proceedings
84. "Finite Size Scaling in Polymer Systems", J. Chem Phys. 88, 5181 (1988)
85. "Molecular Dynamics Studies of Complexing in Binary Molten Salts with Polarizable Ions- MAX_4 " (with M.-L. Saboungi, A. Rahman and M. Blander), J. Chem. Phys. 88, 5818 (1988)
86. "Electronic Structure of Metal-Electrolyte Interfaces: Three- Dimensional Calculation" (with D. L. Price) Phys. Rev. B 38, 9357 (1988)
87. "Theoretical Issues In Electronic Structure of the Passivation Layer" , (proceedings of the German-American colloquium on the passivation layer) Corrosion Science 29,213 (1989)
88. " The Phonon Density of States and the Neutron Scattering Factor for a Disordered Polymer Chain" (with X-L. Chu and K.-L. Yao) Commun. in Theor, Phys. (Beijing, China) 9,253 (1988)
89. "Molecular-dynamics Model for Electron Transfer at the Electrode-Electrolyte Interface" (with J. Hautman), Phys. Rev. B38, 11704 (1988)
90. "Molecular Dynamics Simulation of Water Between Two Ideal Metal Walls" (with J. Hautman and Y-J. Rhee) J. Chem. Phys. 91, 467 (1989)
- 91."Ewald Methods in Molecular Dynamics for Systems of finite Extent in One of Three Dimensions", (with J. Hautman, A. Rahman and Y-J. Rhee) Phys. Rev. B 40,36 (1989)
92. "Many Body Effects in Ion-Water Interactions: Fe^{3+} in Water", (with L. Curtiss and J. Hautman) Chemical Physics 133, 89 (1989)

93. "Absorption of Water in Polymers", (with J.-L. Valles), Journ. of Chem. Phys. 92, 694 (1990)
94. "Electronic Structure of Multiple Vacancies in Rutile TiO_2 by the Equation of Motion Method", (with M. Michalewicz and N. Tit), Phys. Rev. B 41, 10165 (1990)
95. "Estimate of Nuclear Fusion Rates Arising from a Molecular Dynamics Model of PdD_x " (with J. V. Valles) Phys. Rev. B 41, 6072 (1990)
96. "Model for Diffusion with Interactions and Trapping on Realizations of the Percolation Model" (with B. Johnson and J. L. Valles) Physical Review B 42, 4383 (1990)
97. "Numerical Studies of Absorption of Water in Polymers" (with J. L. Valles and B. Johnson) in Computer Simulation Studies in Condensed Matter Physics III, D. P. Landau, K. K. Mon and H. B. Schlutter, Springer-Verlag, Berlin, Heidelberg (1991)
98. "Calculations of the Effects of Point Defects on Hubbard Models of High Temperature Superconductivity", (with S. Davis, R. Joynt and P. Samsel), Bulletin of Materials Science (India) 14, 1069 (1991)
99. "A Mean Field t-J Model for High T_c Containing Two Kinds of Point Defects" (with S. Davis and S. Sen), Physica B 165 & 166, 999 (1990)
100. "Scaling at the Rod-to-Flexible Chain Crossover in the Stiff Limit" (with D. Atkatz and H. Nakanishi), Journ. of Physics A, 23, 3297 (1990)
101. "The Graduate Record Examination as an Indicator of Learning of the Curriculum Taught to Physics Majors in US Institutions", (with A. Adjoudani, P. Heller and J. S. Terwilliger), Am. Journ. of Physics 59, 403 (1991)
102. "Interpretation of Inelastic Light Scattering Measurements in ^4He " (with M. Korth) in "Excitations in 2D and 3D Quantum Fluids", A. F. G. Wyatt and H. J. Lauter, eds. Plenum Press NATO ASI Series B: Physics Vol 257, p. 91 (1991)
103. "Dynamical Properties of the Anderson Localization Model in the Short-Time Critical Regime" (with H. Shore) Physical Review Letters 66, 205 (1991)
104. "Temperature Dependence of the Heterogeneous Ferrous/Ferric Electron Transfer Reaction: Comparison of Experiment and Theory", (with L. A. Curtiss, J. Hautman, N. C. Hung, Z. Nagy, Y. -J. Rhee and R. M. Yonco), Journ. of the Electrochemical Society, 138, 2032 (1991)
105. "Photoelectrochemical Spectroscopy Studies of Anodic Oxides on Titanium: Theory and Experiment", (with M. Kozłowski, M. Michalewicz, W. Smyrl and N. Tit) Surface Science 256, 397 (1991).
106. "Electronic Properties of Disordered TiO_2 Surfaces: Application of the Equation of Motion Method" (with N. Tit and M. Michalewicz), Surface and Interface Analysis 18, 87 (1992).
107. "Scaling of the Insulator to Superconductor Transition in Ultrathin Amorphous Bi Films" (with Y. Liu, A. McGreer, B. Nease, D. B. Haviland, G. Martinez, and A. M. Goldman), Phys. Rev. Letters 67, 2068 (1991)
108. "Point defect Disorder in Models of High Temperature Superconductivity" (with C. Das Gupta, S. Davis and X-F. Wang) Recent Progress in Many Body Theories, Vol

3, T. Ainsworth, C. E. Campbell, B. Clements and E. Krotschek, p.183 (1992), Plenum Press, NY.

109. "Rare-Earth-Iron-Boron Materials in Industrial Applications", in Semiconductors and Rare Earth Based Materials, World Scientific Pub. , Singapore (1991), p.347

110. "Comparison of the Koster-Slater and the Equation of Motion Method for Calculation of the Electronic Structure of Defects in Compound Semiconductors" (with N. Tit), Phys. Rev. B 45, 5887 (1992)

111. "Water Penetration in Glassy Polymers: Experiment and Theory". (with M. Best, B. Johnson and J. L. Valles), Journ. of Applied Polymer Science 48, 319 (1993)

112. "Equation of Motion Method for the Electronic Structure of Disordered Oxides" (with M. Michalewicz, H. Shore and N. Tit), Computer Physics Communications 71, 722(1992)

113. "Mean Field Calculations of the Properties of the Dilute tJ Model for High T_c Superconductivity" (with X-F Wang and S. Davis), Physical Review B46, 6560 (1992)

114. " Jahn-Teller Effect in Liquids: General Principles and a Molecular Dynamics Simulation of the Cupric Ion in Water" (with L. Curtiss and X. R. Wang) Physical Review Letters 69, 2435 (1992)

115. "Phase Diagram of the Two Dimensional Disordered Hubbard Model in the Hartree-Fock Approximation", (with C. Dasgupta), Rapid Comm. of Physical Review B47, 1126 (1993).

116. "Mean Field Predictions of the Dilute tJ Model for High Temperature Superconductivity" (with J. W. Halley, S. Davis and X-F Wang), Condensed Matter Theories, Vol. 8, L. Blum and F. B. Malik, eds. p. 71 (1993),

117. "Role of Oxygen Vacancies in Anodic TiO_2 Thin Films" (with N. Tit and H. Shore) Applied Surface Science 65-6, 246 (1993)

118. "A Polarizable, Dissociating Molecular Dynamics Model for Liquid Water" (with J. R. Rustad and A. Rahman), J. Chem. Phys. 98, 4110 (1993)

119. "Jahn Teller Effect of Cations in Water: The Cupric Ion in Water", (with X. R. Wang and L. Curtiss), in "Models of the Electrode Electrolyte Interface", Electrochemistry Society Proceedings volume 93-5, J.W. Halley and L. Blum eds., The Electrochemical Society, Pennington, N.J. p. 42 (1993)

120. "Calculations of Electronic and Atomic Structure of the Electrode-Electrolyte Interface", (with D. Price), in "Models of the Electrode Electrolyte Interface", Electrochemistry Society Proceedings volume 93-5, J.W. Halley and L. Blum eds., The Electrochemical Society, Pennington, N.J. p. 255 (1993)

121. "Model for the Effects of Phase Separation on Corrosion of Zinc-Nickel Coatings of Steel", , in "Models of the Electrode Electrolyte Interface", Electrochemistry Society Proceedings volume 93-5, J.W. Halley and L. Blum eds., The Electrochemical Society, Pennington, N.J. p. 306 (1993)

122. " Possibility of 2 Types of Localized States in A 2-Dimensional Disordered Lattice"(with N. Tit, N. Kumar and H. Shore) Physical Review B 47, 15988 (1993)

123. "Calculation of Inelastic Light Scattering Spectrum in the Two Body Approximation", (with M. Korth and A. J. Wissink), Phys. Rev. B48, 7399 (1993).
- 124."New Approach to the Observation of the Condensate Fraction in Superfluid Helium Four", (with C. E. Campbell, C. F. Giese and K. Goetz), Physical Review Letters, 71, 2429 (1993).
- 125."Structure of the Condensate in Helium Four and Some Possible Ways to Observe It", Journal of Low Temperature Physics 93, 893 (1993).
- 126." A Novel Approach to the Observation of the Condensate Fraction In Superfluid Helium Four" , Physica B197, 175 (1994)
- 127."Theoretical Analysis of an Experiment to Measure the Condensate Fraction in Superfluid Helium Four" (with C. E. Campbell) Physica B 194-196, 533 (1994)
- 128."Invariance of the Mobility Edge in Anodic Titanium Oxides" (with N. Tit and H. B. Shore) Int'l Journal of Modern Physics B7, 361 (1993)
- 129."Simulation Study of the ferrous-ferric electron transfer at a metal- aqueous electrolyte interface" with B. Smith, J. Chem. Phys. 101, 10915 (1994)
130. "Molecular dynamics simulation of iron(III) and its hydrolysis products in aqueous solution" (with J. R. Rustad and B. P. Hay), Journ. Chem. Phys. 102, 427 (1995)
131. "Electronic Structure of the Passivation Layer: New Computational Methods and Results" (with N. Yu) Materials Science Forum 185-188, 389 (1995)
132. "Jahn Teller Effect of Molecular Complexes in Liquid Solutions" (with X. R. Wang) Modern Physics Letters B8, 1319 (1994)
133. "Test of a Model for the Calculus Based Introductory Physics Course" (with P. J. Ellis) Journal of College Science Teaching, December 1994/January 1995 p. 206 (1994).
134. " Electronic Structure of Point Defects in Rutile" (with N. Yu) Phys. Rev. B51, 4768 (1995)
135. "Molecular Dynamics, Density Functional Theory of the Metal Electrolyte Interface" (with D. L. Price) J. Chem. Phys. 102, 6603 (1995)
136. "A Molecular Dynamics Model of Dimethyl Ether" (with B. Lin) J. Physical Chemistry 99,16474 (1995)
137. "Studies of the Interdependence of Electronic and Atomic Dynamics and Structure at the Electrode-Electrolyte Interface", Electrochimica Acta 41, 2229 (1996)
138. "On the Marcus Model of Electron Transfer at Immiscible Interfaces and Its Application to the Semiconductor/Liquid Interface" (with B. B. Smith and A.J. Nozik) Chemical Physics 205, 245 (1996)
139. " Suspension of Superfluid Helium Using Cesium-Coated Surfaces", (with M. C. Williams and C. F. Giese), Physical Review B 53, 6627 (1996)
140. " A Molecular Dynamics Model of the Amorphous Regions of Polyethylene Oxide" (with B. Lin and P. T. Boinske) J. Chem. Phys. 105, 1668 (1996)

- 141.* "Lithium Ion Transport in a Model of Amorphous Polyethylene Oxide" (with P. T. Boinske, L. Curtiss, B. Lin and A. Sujiatano) *Computer Aided Materials Design* 3, 385 (1996)
142. "Molecular Dynamics Calculation of the Cuprous-Cupric Electron Transfer Reaction at a Copper-Water Interface" (with S. Walbran and B. Smith) *Proceedings of the Conference Electron and Ion Transfer in Condensed Media, Theoretical Physics for Reaction Kinetics*, A. A. Kornyshev, M. Tosi and J. Ulstrup, eds, World Scientific, Singapore (1997) p. 212
143. "Ewald Methods for polarisable Surfaces with Application to Hydroxylation and Hydrogen Bonding on the 012 and 001 Surfaces of α -Fe₂O₃", E. Wasserman J. R. Rustad A. R. Felmy . B. P. Hay and J. W. Halley, *Surface Science* 385, 217 (1997).
144. "What New Models Reveal About the Meaning of Grahame's Capacitance Data" (with A. Mazzolo, S. Walbran and D. L. Price) in " The Electrochemical Double Layer " C. Korzeniewski and B.E. Conway, The Electrochemical Society, Pennington, NJ, Proceedings Volume 97-17 (1997) p. 33
145. "Molecular Dynamics/Electronic Structure Calculations of the Metal-Electrolyte Interface" (with D. L. Price) in " The Electrochemical Double Layer " C. Korzeniewski and B.E. Conway, The Electrochemical Society, Pennington, NJ, Proceedings Volume 97-17 (1997) p. 47
146. "Variational Monte Carlo Studies of the Rate of Transmission of an Atomic Helium Beam Through a Slab of Superfluid Helium by a Condensate Mediated Process" (with A. Setty and C. E. Campbell) , *Phys. Rev. Lett.* 79, 3930 (1997)
147. "Molecular Dynamics Study of the Cu-Water Interface in the Presence of Chlorine" (with Y. Zhou, A. Mazzolo, D.L. Price) *International Journal of Thermophysics* 19, 663 (1998)
148. "First Principles Simulations of the Electrode- Electrolyte Interface" (with A. Mazzolo, Y. Zhou and D. L. Price), *Journal of Interfacial and Electroanalytical Chemistry* 450, 273 (1998)
149. "Experimental and Theoretical Studies of Levitated Quantum Fluids" (with J. Schmidt and C. F. Giese) *Journal of Low Temperature Physics (Kharkov)* 24, 121 (1998)
150. "Self-Consistent tight binding atomic-relaxation model of titanium dioxide" (with P. K. Schelling and N. Yu) *Physical Review B* 58, 1279 (1998)
- 151."Simulation Studies of Polymer Electrolytes for Battery Applications" (with B. Nielsen) *Materials Research Society Proceedings* 496, "Materials for Electrochemical Energy Storage and Conversion II Batteries, Capacitors and Fuel Cells" D.S. Ginley, D.H. Doughty, T. Takamura, Z. Zhang, B. Scrosati, eds.(1998) p.101
152. "Theoretical Modeling of the Solid/Liquid Interface: Chemically Specific Simulation Methods" (with S. Walbran and D.L. Price), "Interfacial Chemistry", A. Wieckowski, editor , Dekker Inc., New York (1999) p.1-18
153. "Model for the electrostatic response of the copper-water interface" (with S. Walbran A. Mazzolo and D. L. Price), *Journal of Chemical Physics* 109, 8076 (1998)
- 154.* "Atomic Structure of Solid and Liquid Polyethylene Oxide", J. Johnson, M-L. Saboungi, D. L. Price, S. Ansell, T. P. Russell, J. W. Halley and B. Nielsen, *Journal of*

Chemical Physics 109, 7005 (1998)

155. "Theory and Experiment on the Cuprous-Cupric Electron Transfer Rate at a Copper Electrode", (with B.B. Smith, S. Walbran, L. A. Curtiss, R. O. Rigney, A. Sujianto, N. C. Hung, R.M. Yonco and Z. Nagy, *Journ. of Chem. Phys.* 110,6538 (1999)

156."Lithium perchlorate ion pairing in a model of amorphous polyethylene oxide" with Y. Duan, L. A. Curtiss and A. G. Baboul, *J. Chem. Phys.* 111, 3302 (1999).

157. "Simulation of battery components and interfaces on the atomic scale: examples of what we can learn", J. W. Halley and Y. Duan, *Journ, of Power Sources* 89, 139 (2000)

158. " Simulation Methods for Chemically Specific Modeling of Electrochemical Interfaces", J. W. Halley, P. Schelling and Y. Duan, *Electrochimica Acta* 46, 239 (2000)

159. "Identical particle scattering from a weakly coupled Bose-Einstein condensed gas" (with A. Wynveen, A. Setty , A. Howard and C. E. Campbell) *Physical Review A* 62, 023602 (2000)

160. "Localization of Polarons: Realistic Calculation in Adiabatic Approximation"(with P. Schelling) *Phys. Rev. B* 62, 3241 (2000)

161. " Chemical Physics of the Electrode-Electrolyte Interface" ", J. W. Halley, S.Walbran and D.L.Price, *Advances in Chemical Physics* 116,337 (2001)

162. " Self Consistent Tight Binding Molecular Dynamics for Realistic Simulation of Oxide Behavior", J. W. Halley, P. K. Schelling and M. Zhuang, in "Proceedings of the Third Recontres du Vietnam: Superconductivity, Magneto-Resistive Materials and Strongly Correlated Systems", Nguyen Van Hieu, Tran Thanh Van and Gang Xiao, eds. Vietnam National University Press (2000) p. 137

163. "Gas Dynamics of Pulsed Low Energy Helium Beams" (with K.Lidke, M. Williams and A. Wynveen) *Journal of Low Temperature Physics* 121, 351 (2000)

164. " Mechanisms of Lithium Conductance in PEO from Molecular Simulation" (with Y. Duan) in " Interfaces, Phenomena, and Nanostructures in Lithium Batteries Workshop , A. Landgrebe, R. J. Klingler eds. ECS proceedings volume 2000-36 (2000) p. 317

165. "Modeling Challenges in Solar Photovoltaic Devices", in *The Global Climate Change: A Coordinated Response by Electrochemistry and Solid-State Science and Technology* , A. Wieckowski, E. W. Brooman, T. F. Fuller, eds. ECS Proceedings Volume 2000-20 (2000) p. 135

166. "Modeling of Semiconductor-Electrolyte Interfaces with Tight Binding Molecular Dynamics" (with P. Schelling) "Solid Liquid Interface; Theory" J. W. Halley, ed. ACS publications (2001) p.142

167. "Direct Dynamics Simulations of the Copper Water Interface: Successes and Problems" (with S. Walbran) "Solid Liquid Interface; Theory" J. W. Halley, ed. ACS publications (2001) p.10

168. "Self Consistent Tight Binding Method for the Prediction of Magnetic Spin Structures in Solids: Application to MnF_2 and MnO_2 " (with Min Zhuang), *Physical Review B* 64, 024413 (2001).

169. "Analysis of photoluminescence experiments on p-type GaAs electrodes using a

- drift diffusion model”, by P Schelling and J. W. Halley, Physical Review B 64, 045326 (2001).
170. "Simulation of polyethylene oxide: Improved structure using better models " (with Yuhua Duan, B. Nielsen, Paul C. Redfern, and Larry A. Curtiss) Journal of Chemical Physics 115, 3957 (2001)
171. "Signatures of Bose-Einstein Condensation in Very Low Energy Atomic Scattering from Trapped Gases", (with A. Wynveen) Laser Physics 12, 223 (2002)
172. "Role of atomic level simulation in development of batteries" (with Y. Duan), Journal of Power Sources 110, 383 (2002)
173. "Multiscale Modeling of Many Body Systems", J. W. Halley, Y. Duan, K. Lidke, A. Wynveen and M. Zhuang, in Condensed Matter Theories Volume 17, M. P. Das and F. Green, editors, Nova Science Publishers, NY (2003) p. 257
174. "Dynamics of low energy helium vapor pulses" A. Wynveen, K.A. Lidke, M.C. Williams, C.F. Giese, J.W. Halley, Phys. Rev. E 67, 026311 (2003)
175. "Self Consistent Direct Dynamics Studies of Interfaces" J. W. Halley, Y. Lin and M. Zhuang, Farad. Discuss, 2002, 212, 85-95
176. "Mechanisms of Lithium Transport in Amorphous Polyethylene Oxide" Yuhua Duan, J. W. Halley, Larry Curtiss, Paul Redfern, J. Chem. Phys. 122, 054702 (2005)
177. "Application of Self Consistent Tight Binding Method to the Study of Anatase Nanocrystals", J. W. Halley, S. Erdin, Y. Lin and Peter Zapol, Proceedings of CMT27, Nova 27th International Workshop on Condensed Matter Theories (CMT-27), SEP 15-20, 2004, Condensed Matter Theories 19, 61-68 (2005)
178. "Helium Vapor Dynamics: Can BEC be produced in a moving frame without confinement?" J. W. Halley, Y. Lutsyshyn and A. Wynveen, Laser Physics 15, 636 (2005)
179. "Phonon Mediated Helium Atom Transmission Through Superfluid Helium Four ", K. A. Lidke, A. Wynveen, N. Baisch, C. Koay, C. F. Giese and J. W. Halley, Journal of Low Temperature Physics 140, 429 (2005)
180. "Self-consistent tight-binding study of low-index titanium surfaces", Serkan Erdin, You Lin and J. Woods Halley, Phys. Rev B 72, 035405 (2005)
181. "Modeling of TiO₂ Nanoparticles" A. S. Barnard, S. Erdin, Y. Lin, P. Zapol and J. W. Halley, Phys. Rev. B 73, 205405 (2006).
182. "Possible Transmission Experiments with Low Velocity Helium Droplets" A. Wynveen, K.A. Lidke, Y. Lutsyshyn and J.W. Halley, Phys. Rev. B 75, 054506 (2007)
183. "Self Consistent Tight Binding Molecular Dynamics Study of TiO₂ Nanoclusters in Water", J. Woods Halley, Serkan Erdin, You Lin, Peter Zapol, Journal of Electroanalytical Chemistry 607, 147 (2007)
184. "Energy Level Statistics of Quantum Dots", Chien-Yu Tsau, Diu Nghiem, R. Joynt and J. Woods Halley, J. Phys.: Condens. Matter 19 (2007) 186215
185. "Proton Transport in HTFSI-EMI-TFSI Mixtures: Experiment and Theory" Lingling Jia, Dat Nguyen, J. W. Halley, Phat Pham, William Lamanna and Steven Hamrock,

Journ. of the Electrochemical Society 156(1) B136-B151 (2009)

186. "Mechanisms of Ionic Transport in Membranes for Batteries and Fuel Cells", J. Woods Halley, Lingling Jia and Sean Bowman, MRS Proceedings / Volume 1269 / 1269-FF03-06 (2010) DOI:10.1557/PROC-1269-FF03-06

187. "A Diffusion Monte Carlo Calculation of the rate of Elastic transmission of a Helium Vapor Beam Through a Slab of Superfluid Helium", Y. Lutsyshyn and J. W. Halley, Phys. Rev. B 83, 014504 (2011)

188. "Relativistic tight-binding model: Application to Pt surfaces", A. Tchernatinsky and J. W. Halley, Phys. Rev. B 83, 205431 (2011).

189."Self consistent tight binding model for dissociable water" You Lin, Aaron Wynveen, J. Halley, Larry Curtiss, and Paul Redfern, Journal of Chemical Physics 136, 174507 (2012)

190. "Use of Magnetite as Anode for Electrolysis of Water", J. W. Halley, A. Schofield and B. Berntson, J. Appl. Phys. 111, 124911 (2012)

191. "Ab Initio Thermodynamic Study of the CO₂ Capture Properties of Potassium Carbonate Sesquihydrate K₂CO₃·1.5H₂O" Yuhua Duan, David Luebke, Henry Pennline, Bingyun Li, Michael Janik, and J. W. Halley, Journal of Physical Chemistry C 116, 14461 (2012)

192. "Hydrogen Generation Using Magnetite to Store Energy from Alternative Sources". J. Woods Halley, Andy Schofield and Bjorn Berntson, CURA Reporter 42, #2, p. 26 (2012).

193. "CO₂ capture properties of lithium silicates with different ratios of Li₂O/SiO₂: an ab initio thermodynamic and experimental approach" Y. Duan, H. Pfeiffer, B. Li, I. C. Romero- Ibarra, D. Sorescu, D. R. Luebke and J. W. Halley, Phys. Chem. Chem. Phys. 15, 13538-13558 (2013), DOI: 10.1039/C3CP51659H

194. "Can Biochemistry Usefully Guide the Search for Better Polymer Electrolytes?", J. Woods Halley, Membranes 2013, 3(3), 242-248; doi:10.3390/membranes3030242

195. "Nonequilibrium steady states in a model for prebiotic evolution" A. Wynveen, I. Fedorov, and J. W. Halley, Phys. Rev. E 89 , 022725 (2014)

196. "Molecular-dynamics calculation of the vacancy heat of transport" Patrick K. Schelling, Jacques Ernotte, Lalit Shokeen, J. Woods Halley, and William C. Tucker, Journal of Applied Physics 116 , 023506 (2014)

197. Yuhua Duan, Jonathan Lekse, Xianfeng Wang, Bingyun Li, Heriberto Pfeiffer, Brenda Alcantar-Vazquez, J. W. Halley "Electronic structure, phonon dynamical properties, and CO₂ capture capability of Na_{2-x}M_xZrO₃ (M = Li, K): Density-functional calculations and experimental validations" Physical Review Applied 3, 044013 (2015) ('Editors' Suggestion') (2015)

198. B. F. Intoy, A. Wynveen, and J. W. Halley, "Effects of spatial diffusion on nonequilibrium steady states in a model for prebiotic evolution", Phys. Rev. E 94, 042424 (2016)

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