

Curriculum Vitae

Gayananath W. Fernando
U-46, 2152, Hillside Rd.,
Physics, Univ. of Connecticut,
Storrs, CT 06269, USA.

Phone: 860-486-0442
Fax: 860-486-3346
gayanath.fernando@uconn.edu
<http://www.phys.uconn.edu>

Education

- 1/85: Ph.D. in Physics, Cornell University, Ithaca, NY 14853, USA.
- 5/82: M.S. in Physics, Cornell University, Ithaca, NY 14853, USA.
- 8/78: B.S. in Mathematics (first class honors) University of Colombo, Sri Lanka.

Work Experience

- 9/91-present: Professor of Physics, Univ. of Connecticut, Storrs, CT 06269, USA.
- 10/87-8/91: Associate and Assistant Scientist in the Physics Department at Brookhaven National Laboratory, Upton, NY 11973, USA.
- 10/86-9/87: Research Associate in the Condensed Matter Theory Group at Brookhaven National Laboratory, Upton, NY 11973, USA.
- 10/84-9/86: Post Doctoral Research Associate with Prof. B. R. Cooper, Dept. of Physics, West Virginia University, Morgantown, WV 26506, USA.
- 6/81-9/84: Graduate Research Assistant with Prof. John W. Wilkins at LASSP, Physics Dept., Cornell University, Ithaca, NY 14853, USA.

Summary of Research Activities

- Worked on a wide variety of problems in theoretical condensed matter, developing accurate theoretical and computational techniques and applying them to examine bulk and surface electronic structure, chemisorption, stability of crystal structures, elastic properties, cohesion, alloy phase diagrams, point defects in alloys, spectroscopic and magnetic properties of transition metal systems, self diffusion in simple liquid metals, and spintronics in heterojunctions.

- Currently working on floquet systems, organic materials and related superconductivity. Recent work on exact many body calculations of Hubbard nanoclusters has uncovered numerous exotic properties of strongly correlated clusters that have not been seen before. Combining exact diagonalization with statistical mechanics has paved the way to a better understanding of phase diagrams, pseudogaps, magnetism and condensation (among other things) of some of the inhomogeneous materials such as the high temperature superconductors and materials exhibiting colossal magnetoresistance.
- Have authored several computer codes for first principles electronic structure and molecular dynamics, Monte Carlo, as well as Embedded Atom Method based studies.

Professional Honors and Other Activities

- Editorial Board, Advances in Condensed Matter Physics
- Published a book on “Metallic Multilayers and their Applications” (publisher: Elsevier 2008)
- Visiting Professor, Nordita, Stockholm, Sweden (July 2019)
- Visiting Professor, Beijing Computational Science and Research Center (Sep.-Oct. 2018)
- Guest Scientist, Brookhaven National Laboratory, USA (1992 - 2015)
- Visiting Professor, Institute of Fundamental Studies, Kandy, Sri Lanka (1997 - 2007)
- Sri Lankan Presidential Award for research carried out in Sri Lanka (Nov. 2001)
- University of Connecticut Summer Research Fellowship (1993)
- Andrew Mellon Fellowship (1980)
- My student, Min Yu, won a Schlumberger Fellowship (2006)
- A co-author of nearly 100 publications in refereed journals. Also a co-author of about a hundred abstracts and presentations at the March Meeting of the American Physical Society (APS), Materials Research Society meeting, Conference on Physical Electronics, American Vacuum Society meeting. Currently refereeing for several journals of the APS.; have also given invited talks at several work shops on recent developments in electronic structure and supervised several Ph.D. thesis projects.

Publications

1. A Brief Review of Electronic and Magnetic Structure of TiF₃, 2440072
<https://doi.org/10.1142/S012915642440072X> July 2024, International Journal of High Speed Electronics and Systems, Gayanath W. Fernando, Donal Sheets, Jason Hancock, Arthur Ernst, R. Matthias Geilhufe
International Journal of High Speed Electronics and Systems 2024 33:02n03
2. Mott insulating negative thermal expansion perovskite TiF₃, Donal Sheets, Kaitlin Lyszak, Menka Jain, **Gayanath W. Fernando**, Ilya Sochnikov, Jacob Franklin, R. Matthias Geilhufe, Jason N. Hancock, arXiv:2311.08382 and Physical Review B 108, 235140 (2023).
3. Correlation Driven Magnetic Frustration and Insulating Behavior of TiF₃, **Gayanath W. Fernando**, Donal Sheets, Jason Hancock, Arthur Ernst, and R. Matthias Geilhufe, arXiv:2310.1264v1 (2023) and Physica Status Solidi (Rapid Research Letters), 2300330 (2023).
4. The Quantumness in Detecting Electromagnetic Waves is Determined by the Interaction Properties of the Detector, C. Roychoudhuri, N. Prasad and **G. Fernando**, Fundamental Research and Application of Physical Science Vol. 3, B P International, Print ISBN: 978-81-19217-29-8, eBook ISBN: 978-81-19217-05-2 (2023),
5. Structural and electronic properties of rare-earth chromites: A computational and experimental study, Jianhang Shi, **Gayanath W. Fernando**, Yanliu Dang, Steven L. Sub and Menka Jain (Phys. Rev. B106, 165117, 2022).
6. Understanding physical processes behind the photoelectric current pulse (PCP) statistics and designing better sources, C. Roychoudhuri, **G. Fernando**, and N. Prasad, Proc. SPIE 12243, Photonics for Quantum 2022, 1224303 (19 July 2022).
7. Driven emergent phases in small interacting condensed-matter systems, **Gayanath W. Fernando**, R. Matthias Geilhufe, Adil-Gerai Kussow and W. Wasanthi P. De Silva, European Physics Letters, Volume 134, 37004 (2021).
8. Multi-hole bands and quasitwo-dimensionality in Cr₂Ge₂Te₆ studied by angle-resolved photoemission spectroscopy, Turgut Yilmaz, Matthias Geilhufe, I. Pletikosic, **G. W. Fernando** et al. European Physics Letters, Volume 133, 27002 (2021).
9. Contrasting quantum sensing light source properties, which generate different photocurrent pulse-statistics, Chandra Roychoudhury, **G. W. Fernando**

nando et al. Proc. of SPIE, Quantum sensing, nano-electronics and photonics XVII, 11288-15 (2020), DOI: 10.1117/12.2551090

10. Chemical-Strain Induced Tilted Dirac Nodes in(BEDT-TTF)₂X₃(X = I, Cl, Br, F) Based Charge-Transfer Salts, R. M. Geilhufe, B. Commeau, and **G. W. Fernando**, Physica Status Solidi (Rapid Research Letters), 1800081 (2018). (DOI: 10.1002/pssr.201800081).
11. Structural and electronic properties of α -(BEDT-TTF)₂I₃, β -(BEDT-TTF)₂I₃ and κ -(BEDT-TTF)₂X₃ (X=I,F,Br,Cl) organic charge transfer salts, B. Commeau, R. M. Geilhufe, **G. W. Fernando**, A. V. Balatsky, Physical Review B **96**, 125135 (2017).
12. From a \mathcal{Z}_2 topological insulator to a square ribbon: Tuning quantum spin Hall states and conductivity, Zhiwei Zhang, Yiteng Tang, and **Gayanath Fernando**, Journal of Applied Physics, **121**, Issue 20, 204302 (2017).
13. Spin-orbit coupling, electron transport and pairing instabilities in two-dimensional square structures, Armen. N. Kocharyan, **Gayanath W. Fernando**, Kun Fang, Kalum Palandage and Alexander V. Balatsky, AIP Advances, **6**, 055711 (2016).
14. Possible phase separation in square and honeycomb Hubbard model: A variational cluster study, Kun Fang, **G. W. Fernando**, A. V. Balatsky and A. N. Kocharyan, Physics Letters A 379, 2230 (2015).
15. Phase separation instabilities and magnetism in two-dimensional square and honeycomb Hubbard model, A. N. Kocharyan, Kun Fang, **G. W. Fernando** and A. V. Balatsky, Journal of Magnetism and Magnetic Materials, **383**, 8 (2015).
16. Phase separation instabilities and pairing modulations in Bi₂Sr₂CaCu₂O_{8+δ}, Kun Fang, **G. W. Fernando**, A. Balatsky, A. N. Kocharyan and K. Palandage, Physics letters A 378, 243 (2014).
17. A Physics Based Lagrangian for the Heat-Diffusion Equation, B. Cassenti, A. Staroselsky and **G. W. Fernando**, Philosophical Magazine Letters, Vol. 93, Issue 5, 307-315 (2013).
18. Nematicity in the two-dimensional one-band Hubbard model, Kun Fang, **G. W. Fernando** and A. N. Kocharyan, J. Phys: Condens. Matter, Vol. 25, 205601 (2013).
19. Quantum Critical Points and Phase Separation Instabilities in Hubbard Nanoclusters, A. N. Kocharyan, **G. W. Fernando** and K. Fang, Journal of Magnetism and Magnetic Materials, **324**, 3427 (2012).
20. Tracing Magnetism and pairing in FeTe-based systems, K. Palandage,

G. W. Fernando, Kun Fang and A. N. Kocharian, Journal of Materials Science, Vol.47, 7671 (2012).

21. Pairing Enhancement in Betts Lattices with Next Nearest Neighbor Couplings; Exact Results, K. Fang, **G. W. Fernando** and A. N. Kocharian, Physics Letters A **376**, 538 (2012)- available online Dec. 2011.
22. A.N. Kocharian, **G.W. Fernando**, and C. Yang, Spin and Charge Pairing Instabilities in Nanoclusters and Nanomaterials, Chapter 15 pp. 507-570 in Scanning Probe Microscopy in Nanoscience and Nanotechnology, ed. by Bharat Bhushan (Springer 2010).
23. Role of point defects on conductivity, magnetism and optical properties in In_2O_3 , Kalum Palandage and **G. W. Fernando**, Physics Letters A **374**, 2879 (2010).
24. Electron coherent and incoherent pairing instabilities in inhomogeneous bipartite and nonbipartite nanoclusters, A. N. Kocharian, **G. W. Fernando**, K. Palandage, and J. W. Davenport, Phys. Lett. A**373**, 1074-1082 (2009).
25. Pairing in bipartite and nonbipartite repulsive Hubbard clusters: Octahedron, **G. W. Fernando**, K. Palandage, A. N. Kocharian and J. W. Davenport, Physical Review B **80**, 014525 (2009); *Selected to appear in the virtual journal of nanotechnology*.
26. An energy conservation approach to adsorbate-induced surface stress and the extraction of binding energy using nanomechanics, L. A. Pin naduwage, V. I. Boiadzhiev, J. E. Hawk, A. C. Gehl, **G. W. Fernando** and L. C. R. Wijewardhana, Nanotechnology, **19**, 105501 (2008)
27. Coherent and incoherent pairing instabilities and spin charge separation in bipartite and nonbipartite nanoclusters: Exact results, A. N. Kocharian, **G. W. Fernando**, K. Palandage and J. W. Davenport Physical Review B **78**, 075431 (2008)
28. Exact Thermodynamics of pairing and charge spin separation crossovers in small Mott-Hubbard nanoclusters, A. N. Kocharian, **G. W. Fernando**, T. Wang, K. Palandage and J. W. Davenport, Physics Letters A, **364**, 57 (2007)
29. Phase separation and electron pairing in repulsive Hubbard Clusters, **G. W. Fernando**, A. N. Kocharian, K. Palandage, Tun Wang and J. W. Davenport, Physical Review B **75**, 085109 (2007)
30. Discrete size series of CdSe quantum dots: A combined computational and experimental investigation, M. Yu, **G. W. Fernando**, R. Li, F.

Papadimitrakopoulos, N. Shi and R. Ramprasad, Journal of Computer-Aided Materials Design, **14**, 167 (2007)

31. Exact study of pairing fluctuations and phase diagrams in 4-site Hubbard nanocluster, K. Palandage, **G. W. Fernando**, A. N. Kocharian, J. W. Davenport, Journal of Computer-Aided Materials Design, **14**, 103 (2007)
32. First principles study of CdSe quantum dots: Stability, surface unsaturations and experimental validation, M. Yu, G. W. Fernando, R. Li, F. Papadimitrakopoulos, N. Shi and R. Ramprasad, *Applied Physics Letters*, **88**, 231910 (2006)
33. An exact study of charge-spin separation, pairing fluctuations and pseudogaps in 4-site Hubbard clusters, A. N. Kocharian, G. W. Fernando, K. Palandage and J. W. Davenport, *Physical Review B* **74**, 024511 (2006)
34. Thermodynamic properties, Magnetism and Mott-Hubbard like Transitions in Nanoscale Clusters, A. N. Kocharian, G. W. Fernando, K. Palandage and J. W. Davenport, *Journal of Magnetism and Magnetic Materials*, 300, e585 (2006); available online since Nov. 2005
35. H. Zhang, J. Gromek, G. Fernando, R. S. Boorse and H. L. Marcus, Study of Novel Nanostructured Pd-Mn Oxides, *Physica B*, Vol. 344, 278 (2004)
36. Reduction of the 3 Dimensional Schrödinger Equation for Multilayered Films, C. Abbott, G. W. Fernando, and M. Rasamny, *Physical Review B* **69**, 205412 (2004)
37. H. Zhang, J. Gromek, G. Fernando, and H. L. Marcus, Novel Nanostructured Pd-Zr Oxides, *Mat. Sci. and Engineering*, A366, 248 (2004)
38. PdO/Pd System equilibrium phase diagram, by H. Zhang, J. Gromek, G. W. Fernando, S. Boorse and H. Marcus, *Journal of Phase Equilibria*, 23, 246 (2002)
39. Density Functional Theory and Atomic Multiplet Levels, M. Weinert, R. E. Watson and G. W. Fernando, *Physical Review A* **66**, 032508 (2002)
40. Electronic Structure and Thermodynamics of Defects in NiAl₃, by M. Rasamny, M. Weinert, G. W. Fernando and R. E. Watson, *Physical Review B* **64**, 144107 (2001)
41. H. Zhang, J. Gromek, M. Augustine, G. Fernando, M. Rasmany, R. S. Boorse and H. L. Marcus In-Situ High-Temperature X-Ray Study of Al₂O₃ Supported PdO Catalyst, Published in Powder Materials:: Current Research and Industrial Practice, The Minerals, Metals and Materials Society, p 59, 2001

42. H. Zhang, J. Gromek, M. Augustine, G. W. Fernando, R. S. Boorse and H. L. Marcus, Synthesis and Characterization of Novel Pd-Mn Oxides, published in MRS Proceedings, Fall Meeting 2001
43. Magnetic Moment of Iron in Metallic Environments by G. W. Fernando, R. E. Watson, M. Weinert, A. N. Kocharian, A. Ratnaweera and K. Tennakone, *Physical Review B* **61**, 375 (2000)
44. Theoretical Study of Relativistic Effects in the Electronic Structure of Plutonium by G. W. Fernando, E. H. Sevilla and B. R. Cooper, *Physical Review B* **61**, 12562 (2000)
45. Interatomic Potentials via the Effective Action Formalism by M. F. Rasamny, M. Valiev, and G. W. Fernando, *Physical Review B* **58**, 9700 (1998)
46. Stoner Criterion of Ferromagnetism and Moment Saturation in the Hubbard Model with an Applied Magnetic Field by G. W. Fernando, A. N. Kocharian, R. E. Watson, and M. Weinert, *Physica B*, **230-232**, 509 (1997)
47. Density Functional Theory of One Electron Propagators by M. Valiev and G. W. Fernando, *Physics Letters A*, **227**, 265 (1997)
48. Path Integral Formulation of Exchange-Correlation Energy by M. Valiev and G. W. Fernando *Physical Review B* **54**, 7765 (1996)
49. NMR study of Y_2Fe_{17} Nitrides by Y. D. Zhang, J. I. Budnick, N. X. Shen, W. A. Hines, G. W. Fernando, and T. Manzur, *Journal of Magnetism and Magnetic Materials* **987**, 141 (1995)
50. Nitrogen Diffusion Behavior in the Y_2Fe_{17} Lattice by Y. D. Zhang, D. P. Yang, J. I. Budnick, G. W. Fernando, T. D. Xiao and T. Manzur *Physical Review B* **51**, 12091 (1995)
51. Occupation Numbers in Density Functional Calculations by M. Valiev and G. W. Fernando *Physical Review B* **52**, 10697 (1995)
52. Point Group Symmetries and Gaussian Integration by G. W. Fernando, M. Weinert, R. E. Watson and J. W. Davenport, *Journal of Computational Physics*, Vol. 112, No. 2, 282 (1994)
53. Alloy Heats of Formation: Theory vs Experiment by R. E. Watson, M. Weinert, J. W. Davenport and G. W. Fernando, *Journal Phase Equilibria*, Vol. 15, 273 (1994)
54. The Energetics of Ordered Intermetallic Alloys (of the Transition Metals) by R. E. Watson, M. Weinert, J. W. Davenport, G. W. Fernando, and L. H. Bennett - Statics and Dynamics of Alloy Phase Transitions, Edited by P. E. A. Turchi and A. Gonis, Plenum Press, New York, 1994

55. Surface Electronic Structure of γ Uranium by Y. G. Hao, O. Eriksson, G. W. Fernando and B. R. Cooper, *Physical Review B* **47**, 6680 (1993)
56. Cu-Pd multilayers: Embedded Atom and First Principles Calculations, by G. W. Fernando, J. Mei, R. E. Watson, M. Weinert, and J. W. Davenport, *Physical Review B* **47**, 13636 (1993)
57. Possibility of a δ -like surface for α -Pu: Theory by O. Eriksson, L. E. Cox, B. R. Cooper, J. M. Wills, G. W. Fernando, Y. G. Hao, and M. Boring, *Physical Review B* **46**, 13576 (1992)
58. The energetics of ordered intermetallic alloys, by R. E. Watson, M. Weinert, J. W. Davenport, G. W. Fernando and L. H. Bennett, Proc. NATO Advanced Study Institute on Statics and Dynamics of Alloy Phase Transformations, Rhodes, Greece, June-July 1992.
59. On Prediction of Ferromagnetism and Metamagnetism in 4d Transition-Metal Overlayers, by O. Eriksson, R. C. Albers, A. M. Boring, G. W. Fernando and B. R. Cooper, *Modern Physics Letters* **B6**, 605 (1992)
60. The Heats of Formation of Transition Metal Alloys: Pt-Ti system by G. W. Fernando, R. E. Watson and M. Weinert, *Physical Review B* **45**, 8233 (1992)
61. First Principles Calculations: The Elemental Transition Metals and Their Compounds by R. E. Watson, G. W. Fernando, M. Weinert and J. W. Davenport, *Journal of Phase Equilibria* **13**, 244 (1992)
62. Surface Electronic Structure and Chemisorption of Plutonium and Uranium by B. R. Cooper, O. Eriksson, Y. G. Hao and G. W. Fernando, Transuranium Elements - A Half Century, Chapter 36, 365 (1992) - published by the American Chemical Society.
63. Spin and Orbital Contributions to Surface Magnetism in 3d Elements by O. Eriksson, A. M. Boring, R. C. Albers, G. W. Fernando and B. R. Cooper, *Physical Review B* **45** 2868 (1992)
64. Cohesion and Promotion Energies in Transition Metals: Implications of the local density Approximation by R. E. Watson, G. W. Fernando, M. Weinert, Y. J. Wang and J. W. Davenport, *Journal of Applied Physics* **69**, 5688 (1991)
65. The Local Density Approximation: Cohesion in the Transition Metals and $s \rightarrow d$ Promotion in the Transition Metal Atoms by R. E. Watson, G. W. Fernando, M. Weinert, Y. J. Wang and J. W. Davenport, *Physical Review B* **43**, 1455 (1991)
66. Charge Transfer in Transition Metal Alloying: Charge Tailing Effects by

- R. E. Watson, M. Weinert and G. W. Fernando, *Physical Review B***43**, 1446 (1991)
67. Surface Electronic Structure of Ce in the α and γ Phases by O. Eriksson, R. Albers, M. Boring, G. W. Fernando, Y. G. Hao and B. R. Cooper, *Physical Review B***43**, 3137 (1991)
68. Theoretical Studies of Electronic Structure of Hydrogen and Oxygen Chemisorbed on Pu by O. Eriksson, Y. G. Hao, B. R. Cooper, G. W. Fernando, L. E. Cox, J. M. Ward, and A. M. Boring, *Physical Review B***43**, 4590 (1991)
69. Analytic Embedded Atom potentials by J. Mei, J. W. Davenport and G. W. Fernando, *Physical Review B***43**, 4653 (1991)
70. Electronic structure of the (111) and (100) Surfaces of δ -Pu by Y. G. Hao, O. Eriksson, G. W. Fernando and B. R. Cooper *Physical Review B***43**, 9467 (1991)
71. Anomalies in the Elastic Properties of Metallic Multilayers by J. Mei and G. W. Fernando, *Physical Review Letters* **66**, 1882 (1991)
72. Enhanced Orbital Contribution to Surface Magnetism in Fe, Co and Ni by O. Eriksson, G. W. Fernando, R. C. Albers, and A. M. Boring *Solid State Communications* **78**, 801 (1991)
73. Charge Transfer, Charge Tailing, Cohesion and Electron Promotion in the Transition Metals by R. E. Watson, M. Weinert, G. W. Fernando, J. W. Davenport *Physica* **B172**, 289 (1991)
74. Energetics of Metal-Metal Interfaces by M. Weinert, R. E. Watson, J. W. Davenport and G. W. Fernando. Ordering at Surfaces and Interfaces, Springer-Verlag, Berlin, 1990 (Conference Proceedings)
75. Iterative Approaches to Electronic Structure with Augmented Bases by G. W. Fernando, *Physical Review B***41**, 903 (1990)
76. Cohesion and Lattice Stabilities in the 5d Transition Metals by G. W. Fernando, R. E. Watson, M. Weinert, J. Wang, and J. W. Davenport, *Physical Review B***41**, 11813 (1990)
77. First Principles Calculation of the Activation Energy for Diffusion in Liquid Sodium by G-X. Qian, M. Weinert, G. W. Fernando and J. W. Davenport, *Physical Review Letters* **64**, 1146 (1990)
78. Electronic Structure of NiAl by S. -C. Liu, J. W. Davenport, E. W. Plummer, D. M. Zehner and G. W. Fernando, *Physical Review B***42**, 1582 (1990)

79. First Principles Molecular Dynamics Studies of Liquid and Solid Sodium by J. W. Davenport, G.-X. Qian, G. W. Fernando and M. Weinert, *The Int. Journal of Supercomputer Applications*, Vol 4, No. 3, 122 (1990)
80. Electronic Structure of Transition Metal Alloys and Intermetallics: Charge Transfer and Its Implications for Mössbauer Effect Measurements by R. E. Watson, J. W. Davenport, M. Weinert and G. W. Fernando, *Hyperfine Interactions* **53**, 213 (1990)
81. Energetics of Metal-Metal Interfaces by M. Weinert, R. E. Watson, J. W. Davenport and G. W. Fernando. *Ordering at Surfaces and Interfaces*, Springer-Verlag, Berlin, 1990 (Conference Proceedings)
82. Antiferromagnetism of CuO₂ Layers by M. Weinert and G. W. Fernando, *Physical Review B* **39**, 835 (1989) - rapid communications
83. Full Potential LASTO by G. W. Fernando, J. W. Davenport, R. E. Watson and M. Weinert, *Physical Review B* **40**, 2757 (1989)
84. Adsorbed layer and multilayer materials: The Energetics and Bonding of Pd-Nb(100), Pd-Nb(110) and Ag-Nb(110) by M. Weinert, R. E. Watson, J. W. Davenport and G. W. Fernando, *Physical Review B* **39**, 12585 (1989)
85. Surface Electronic Behavior of Actinide Metals by Y. G. Hao, G. W. Fernando and B. R. Cooper, *Journal of Vacuum Science and Technology A* **7**, 2065 (1989)
86. The Energetics of Transition Metal Alloy Formation: Ti, Zr and Hf Alloyed with the Heavier 4d and 5d Elements by R. E. Watson, M. Weinert, J. W. Davenport and G. W. Fernando, *Physical Review B* **39**, 10761 (1989)
87. First Principles Molecular Dynamics for Metals by G. W. Fernando, Guo-Xin Qian, M. Weinert and J. W. Davenport, *Physical Review B* **40**, 7985 (1989)
88. Structural Stability of Rhenium as a Function of Lattice Compression: Theory by R. E. Watson, J. W. Davenport, M. Weinert and G. W. Fernando, *Physical Review B* **38**, 7817 (1988)
89. The Energetics of Transition Metal Alloy Formation: Theory versus Experiment by R. E. Watson, M. Weinert, J. W. Davenport and G. W. Fernando, *Scripta Metallurgica* **22**, 1285 (1988)
90. Localized States at Metal-Metal Interfaces: An Inverse Photoemission Study by X. Pan, P. D. Johnson, M. Weinert, R. E. Watson, J. W. Davenport, G. W. Fernando and S. L. Hulbert, *Physical Review B (rapid communications)* **38**, 7850 (1988)

91. Theory of Electronic Structure and Magnetic Behavior of fcc Iron Grown on Cu(001) by G. W. Fernando and B. R. Cooper, *Physical Review B* **38**, 3016 (1988)
92. Two Magnetically Different States of fcc Fe grown on Cu(100) by P. A. Montano, G. W. Fernando, B. R. Cooper, E. R. Moog, H. M. Naik, S. D. Bader, Y. C. Lee, Y. N. Darici, H. Min and J. Marcano, *Physical Review Letters* **59**, 1041 (1987)
93. Electronic Structure of fcc Iron Grown on Copper by G. W. Fernando, Y. C. Lee, P. A. Montano, B. R. Cooper, E. R. Moog, H. M. Naik and S. D. Bader, *Journal of Vacuum Science and Technology A5*, 882 (1987)
94. Systematics in Bonding of Simple Adsorbates on a Transition Metal Surface by G. W. Fernando and J. W. Wilkins, *Physical Review B* **35**, 2995 (1987)
95. A LAPW Study of Chemisorption of Sulfur on Fe(001) by G. W. Fernando and J. W. Wilkins, *Physical Review B* **33**, 3709 (1986)
96. Practical Method for Highly Accurate Large Scale Surface Calculations by G. W. Fernando, B. R. Cooper, M. V. Ramana, H. Krakauer and C. Q. Ma, *Physical Review Letters* **56**, 2299 (1986)