

PUBLICATIONS

1. O. Gunnarsson, B.I. Lundqvist and S. Lundqvist: Screening in a Spin Polarized Electron Liquid. *Solid State Commun.* **11**, 149 (1972).
2. G. Grimvall and O. Gunnarsson: Concepts in Many-Body Systems Illustrated by Coupled Oscillators. *Am J. Phys.* **41**, 1241 (1973).
3. O. Gunnarsson, B.I. Lundqvist and J.W. Wilkins: Contribution to the Cohesive Energy of Simple Metals: Spin-Dependent Effect. *Phys. Rev.* **B 10**, 1319 (1974).
4. O. Gunnarsson and H. Hjelmberg: Hydrogen Chemisorption by the Spin-Density-Functional Formalism. *Physica Scripta* **11**, 97 (1975).
5. O. Gunnarsson, P. Johansson, S. Lundqvist and B.I. Lundqvist: Chemical Binding in Small Molecules by the Spin-Density-Functional Formalism. *Int. J. Quant. Chem.* **9S**, 83 (1975).
6. O. Gunnarsson and P. Johansson: The Spin-Density-Functional Formalism for Quantum Mechanical Calculations: Test on Diatomic Molecules with an Efficient Numerical Method. *Int. J. Quant. Chem.* **10**, 307 (1976).
7. O. Gunnarsson: Band Model for Magnetism of Transition Metals in the the Spin-Density-Functional Formalism. *J. Phys. F* **6**, 587 (1976).
8. O. Gunnarsson and B.I. Lundqvist: Exchange and Correlation in Atoms, Molecules and Solids by the Spin-Density-Functional Formalism. *Phys. Rev.* **B13**, 4274 (1976).
9. O. Gunnarsson, J. Harris and R.O. Jones: Cluster Calculations using Muffin-Tin Orbitals. *J. Phys. C* **9**, 2739 (1976).
10. O. Gunnarsson, H. Hjelmberg and B.I. Lundqvist: Binding Energies for Different Adsorption Sites of Hydrogen on Simple Metals. *Phys. Rev. Lett.* **37**, 292 (1976).

11. O. Gunnarsson, M. Jonson and B.I. Lundqvist: Exchange and Correlation in Atoms, Molecules and Solids. *Phys. Lett.* **59A**, 177 (1976).
12. O. Gunnarsson, H. Hjelmberg and B.I. Lundqvist: Calculation of Geometries and Chemisorption Energies of Adatoms on Simple Metals. *Surf. Sci.* **63**, 348 (1977).
13. O. Gunnarsson, J. Harris and R.O. Jones: Muffin-Tin Orbitals and the Total Energy of Atomic Clusters. *Phys. Rev.* **B15**, 3027 (1977).
14. O. Gunnarsson: The Stoner Model in the Spin-Density-Functional Formalism. Invited paper to the EPS conference on Itinerant-Electron Magnetism, Oxford 1976. *Physica* **91BC**, 329 (1977).
15. O. Gunnarsson, J. Harris and R.O. Jones: Molecular Calculations using the Muffin-Tin Orbital Method. *Int. J. Quant. Chem.* **11S**, 71 (1977).
16. H. Hjelmberg, O. Gunnarsson and B.I. Lundqvist: Theoretical Studies of Atomic Adsorption on Nearly-Free-Electron-Metal Surfaces. *Surf. Sci.* **68**, 158 (1977).
17. O. Gunnarsson, J. Harris and R.O. Jones: Density-Functional Theory and Molecular Bonding. First-row Diatomic Molecules. *J. Chem. Phys.* **67**, 3970 (1977).
18. K. Schönhammer and O. Gunnarsson: Relaxation Shifts in Adsorbate Levels. *Proc. 7th Int. Vac. Congr. and 3rd Conf. Solid Surfaces.* (Vienna 1977) p. 795.
19. B.I. Lundqvist, H. Hjelmberg and O. Gunnarsson: Adsorbate-Induced Electronic States in *Photoemission and the Electronic Properties of Surfaces* edited by B. Feuerbacher, B. Fitton R.F. Willis (Wiley, New York, 1978) p. 227.
20. K. Schönhammer and O. Gunnarsson: Shape of Core Level Spectra in Adsorbates. *Solid State Commun.* **23**, 691 (1977).
21. O. Gunnarsson, M. Jonson and B.I. Lundqvist: Exchange and Correlation in Inhomogeneous Electron Systems. *Solid State Commun.* **24**, 765 (1977).

22. K. Schönhammer and O. Gunnarsson: Correlation Effects on Core Level Spectra of Adsorbates. *Solid State Commun.* **26**, 399 (1978).
23. O. Gunnarsson: Band Magnetism in the Spin-Density-Functional Formalism. Invited paper at the 23rd annual conf. on Magnetism and Magnetic Materials. *J. Appl. Phys.* **49**, 1399 (1978).
24. O. Gunnarsson and K. Schönhammer: Plasmon Effects on Core Level Spectra of Adsorbates. *Solid State Commun.* **26**, 147 (1978).
25. K. Schönhammer and O. Gunnarsson: Exactly Soluble Limits of a Model for Core Level Spectra of Adsorbates. *Z. Phys.* **B30**, 297 (1978).
26. O. Gunnarsson and K. Schönhammer: Time-Dependent Approach to the Calculation of Spectral Functions. *Phys. Rev.* **B18**, 6606 (1978).
27. O. Gunnarsson and K. Schönhammer: CO on Cu(100) - Explanation of the Three-Peak Structure in the X-ray-Photoemission- Spectroscopy Core Spectrum. *Phys. Rev. Lett.* **41**, 1608 (1978); **42**, 195 (1979).
28. O. Gunnarsson and K. Schönhammer: Shape of Core Level Spectra in Adsorbates. *Surf. Sci.* **80**, 471 (1979).
29. O. Gunnarsson: Density Functional Theory of Metallic Surfaces. Lectures at the NATO Advanced Study Institute *Electrons in Disordered Metals and at Metallic Surfaces* edited by P. Phariseau, B.L. Györfy and L. Scheire (Plenum, New York, 1979) p. 1.
30. O. Gunnarsson, M. Jonson and B.I. Lundqvist: Descriptions of Exchange and Correlation Effects in Inhomogeneous Electron Systems. *Phys. Rev.* **B20**, 3136 (1979).
31. B.I. Lundqvist, O. Gunnarsson, H. Hjelmberg and J. Norskov: Theoretical Description of Molecule-Metal Interaction and Surface Reactions. Invited paper at ECOSS 2,

- Camebridge 1979. Surf. Sci. **89**, 196 (1979).
32. K. Schönhammer and O. Gunnarsson: Many-Body Effects in Deep Level Spectroscopy from Adsorbates. Invited paper at ECOSS 2, Camebridge 1979, Surf. Sci. **89**, 575 (1979).
 33. O. Gunnarsson and R.O. Jones: Density Functional Calculations for Atoms, Molecules and Clusters. Invited paper at the 46th Nobel Symposium. Physica Scripta **21**, 394 (1980).
 34. O. Gunnarsson and K. Schönhammer: Many-Body Effects in XPS for Adsorbed Atoms and Molecules. Invited paper at the 46th Nobel Symposium. Physica Scripta **21**, 575 (1980).
 35. O. Gunnarsson, H. Hjelmberg and J.K. Norskov: Variation of Adatom Valence-Level Positions with the Distance to a Metal Surface. Physica Scripta **22**, 165 (1980).
 36. J.C. Fuggle, R. Lässer, O. Gunnarsson and K. Schönhammer: Plasmon Gains as Monitor of Incomplete Relaxation, Interference Effects, and the Transition from Sudden to Adiabatic Limits in Electron Spectroscopies. Phys. Rev. Lett. **44**, 1090 (1980).
 37. O. Gunnarsson and R.O. Jones: Extension of the LSD Approximation in Density Functional Calculations. J. Chem. Phys. **72**, 5357 (1980).
 38. O. Gunnarsson and K. Schönhammer: Comment on "Negative Shake-up Energy in Core Ionization". Phys. Rev. **B21**, 5863 (1980).
 39. K. Schönhammer and O. Gunnarsson: Localized Dynamic Perturbations in Metals. Z. Phys. **B38**, 127 (1980).
 40. K. Schönhammer and O. Gunnarsson: Sticking Probability on Metal Surfaces: Contribution from Electron-Hole Pair Excitations. Phys. Rev. **B22**, 1629 (1980).

41. O. Gunnarsson and K. Schönhammer: Dynamical Theory of Auger Processes. *Phys. Rev.* **B22**, 3710 (1980).
42. O. Gunnarsson and K. Schönhammer: One-Step Description of XPS and Auger Spectra. *Le Vide, Les Couces Minces* **4**, 172 (1980).
43. O. Gunnarsson and R.O. Jones: Self-Interaction Corrections in the Density Functional Formalism. *Solid State Commun.* **37**, 249 (1981).
44. O. Gunnarsson and K. Schönhammer: Additional Information in Auger-Electron-Photo-electron Coincidence Spectroscopy? *Phys. Rev. Lett.* **46**, 859 (1981).
45. O. Gunnarsson, K. Schönhammer, J.C. Fuggle and R. Lässer: Interference Effects in Auger Electron Spectroscopy. *Phys. Rev.* **B23**, 4350 (1981).
46. K. Schönhammer and O. Gunnarsson: Sticking Probability on Metal Surfaces. Temperature-Dependence of the Electron-Hole Pair Mechanism. *Phys. Rev.* **B24**, 7084 (1981).
47. O. Gunnarsson and K. Schönhammer: Boson Approximations for Localized Dynamic Perturbations in Metals. *Phys. Rev.* **B25**, 2503 (1982).
48. O. Gunnarsson and K. Schönhammer: Inelastic Scattering of Rare-Gas Atoms from Metal Surfaces. Excitation of Electron-Hole Pairs. *Phys. Rev.* **B25**, 2514 (1982).
49. O. Gunnarsson and K. Schönhammer: Electronic Aspects of Adsorption Rates. Invited talk at the International Summer Institute in Surface Science 1981 in Milwaukee. *Springer Series in Chemical Physics*. Vol. 20, p. 363 (1982).
50. K. Schönhammer and O. Gunnarsson: Sticking and Inelastic Scattering at Metal Surfaces: The Electron-Hole Pair Mechanism. *Surf. Sci.* **117**, 53 (1982).
51. O. Gunnarsson and K. Schönhammer: Interpretation of X-Ray Photoelectron Spectra for Large Systems. *Phys. Rev.* **B26**, 2765 (1982).

52. K. Schönhammer and O. Gunnarsson: One-Step Description of XPS and Auger Processes. Invited talk at the 2nd Conf. of the Condensed Matter Division of the European Physical Society, Manchester. *Physica Scripta* **T1**, 115 (1982).
53. O. Gunnarsson and K. Schönhammer: One-Step Model of X-Ray Photoemission and Auger Processes. Invited paper at the Int. Conf. on X-ray and Atomic Inner-Shell Physics, Eugene, Oregon, 1982. *AIP Conf. Proceedings* **94**, 517 (1982).
54. O. Gunnarsson and R.O. Jones: Exchange-Correlation Energy Functionals in the Density Functional Formalism in *Local Density Approximations in Quantum Chemistry and Solid State Theory*. Edited by J.P. Dahl and J. Avery (Plenum, New York, 1983) p. 229.
55. K. Schönhammer and O. Gunnarsson: Energy Dissipation at Metal Surfaces: Electronic versus Vibrational Excitations. Invited talk at *Vibrations at Surfaces*, 3rd Int. Conf. at Asilomar, California 1982. *J. Elec. Spectr.* **29**, 91 (1983).
56. K. Schönhammer and O. Gunnarsson: Electronic Friction and Covalent Chemisorption. *Phys. Rev.* **B27**, 5113 (1983).
57. O. Gunnarsson and K. Schönhammer: Photoemission from Ce Compounds - Exact Model Calculation in the Limit of Large Degeneracy. *Phys. Rev. Lett.* **50**, 604 (1983).
58. J.C. Fuggle, F.U. Hillebrecht, J.-M. Esteve, R.C. Karnatak, O. Gunnarsson and K. Schönhammer: f-count Effects in X-Ray Absorption Spectra of the 3d Level in Ce and its Compounds. *Phys. Rev.* **B27**, 4637 (1983).
59. J.C. Fuggle, F.U. Hillebrecht, Z. Zolnierok, R. Lässer, Ch. Freiburg, O. Gunnarsson and K. Schönhammer: Electronic Structure of Ce and its Intermetallic Compounds. *Phys. Rev.* **B27**, 7330 (1983).
60. O. Gunnarsson, O. Jepsen and O.K. Andersen: Self-Consistent Impurity Calculations in the Atomic-Spheres Approximation. *Phys. Rev.* **B27**, 7144 (1983).

61. O. Gunnarsson and K. Schönhammer: Electron Spectroscopies for Ce Compounds in the Impurity Model. *Phys. Rev.* **28**, 4315 (1983).
62. O. Gunnarsson, K. Schönhammer, J.C. Fuggle, F.U. Hillebrecht, J.-M. Esteve, R.C. Karnatak and B. Hillebrand: The Occupancy and Hybridization of the f-Level in Ce Compounds. *Phys. Rev.* **B28**, 7330 (1983).
63. F.U. Hillebrecht, J.C. Fuggle, G.A. Sawatzky, M. Campagna, O. Gunnarsson and K. Schönhammer: Transition to Nonmagnetic f-states in Ce Intermetallic Compounds studied by Brems-Strahlung Isochromat Spectroscopy (BIS). *Phys. Rev.* **B30**, 1777 (1983).
64. O. Gunnarsson and K. Schönhammer: Aspects of Core Level X-Ray Photoemission for Large Systems in *Many-Body Phenomena at Surfaces* edited by D. Langreth and H. Suhl Academic, Orlando, 1984) p. 221. Invited talk at the workshop “Many-body phenomena at surfaces”, Santa Barbara, July 18-29, 1984.
65. K. Schönhammer and O. Gunnarsson: Energy Dissipation at Metal Surfaces: The Electron-Hole Pair Mechanism in *Many-Body Phenomena at Surfaces* edited by D. Langreth and H. Suhl Academic, Orlando, 1984) p. 421.
66. O. Gunnarsson and K. Schönhammer: Model Calculations of Electron Spectra for Ce Mixed Valence Compounds in *Moment Formation in Solids* edited by W.J.L. Buyers. NATO ASI series Vol. 117 (Plenum, New York, 1984) p. 289.
67. K. Schönhammer and O. Gunnarsson: Local Polaron Effects in Mixed Valence Systems: Exact Model Calculation in the Limit of large Degeneracy. *Phys. Rev.* **30**, 3141 (1984).
68. O. Gunnarsson and K. Schönhammer: Double Occupancy of the f-level in the Anderson Model for Ce Compounds. *Phys. Rev.* **B31**, 4815 (1985).

69. K. Schönhammer and O. Gunnarsson: Energy Dissipation at Metal Surfaces: The Electron-Hole Pair Mechanism. Invited talk at the 7th Taniguchi Symposium *Dynamical Processes and Ordering on Solid Surfaces*. Edited by A. Yoshimori and M. Tsukada, Springer Series in Solid State Physics. Vol. 59, p. 57 (1985).
70. O. Gunnarsson and K. Schönhammer: Double Occupancy in the Anderson Model. *J. Magn. Magn. Mater.* **47-48**, 266 (1985).
71. K. Schönhammer and O. Gunnarsson: Local Polaron Effects in Mixed Valence Systems. *J. Magn. Magn. Mater.* **47-48**, 309 (1985).
72. O. Gunnarsson and R.O. Jones: Total Energy Differences: Sources of Error in Local Density Approximations. *Phys. Rev.* **B31**, 7588 (1985).
73. O. Gunnarsson, K. Schönhammer, D.D. Sarma, F.U. Hillebrecht and M. Campagna: Core Level Spectra of Th Compounds. *Phys. Rev. (Rapid Commun.)* **B32**, 5499 (1985).
74. F. Beeler, M. Scheffler, O. Jepsen and O. Gunnarsson: Identification of Chalcogen Point-Defect Sites in Silicon by Total Energy Calculations. *Phys. Rev. Lett.* **54**, 2525 (1985).
75. R.O. Jones and O. Gunnarsson: Density-Functional Formalism: Sources of Error in Local Density Approximations. *Phys. Rev. Lett.* **55**, 107 (1985).
76. M. Scheffler, F. Beeler, O. Jepsen, O. Gunnarsson, O.K. Andersen and G.B. Bachelet: Chemical Bonding and Lattice Relaxations of Deep Level Defects. Proceedings of 13th International Conf. on Defects in Semiconductors. Eds.: L.C. Kimerling and J.M. Parsey. The Metallurgical Society of AIME Conference Proceedings, p. 45 (1985).
77. O. Gunnarsson and K. Schönhammer: The frequency-Dependent Susceptibility in the Anderson Model. Invited talk at 8th Taniguchi Symposium *Theory of Heavy Fermions*

and Valence Fluctuations. Edited by T. Kasuya and T. Saso, Springer Series in Solid State Physics. Vol 62, p. 100 (1985).

78. O. Gunnarsson and K. Schönhammer: Ground-State and Spectroscopic Properties of the Finite U Anderson Model. Invited talk at the 8th Taniguchi Symposium *Theory of Heavy Fermions and Valence Fluctuations*. Edited by T. Kasuya and T. Saso, Springer Series in Solid State Physics. Vol 62, p. 110 (1985).
79. O. Gunnarsson and K. Schönhammer: Spectroscopic Properties of Mixed Valence Compounds in the Impurity Model. Invited talk at the 5th Int. Conference on Crystalline Field and Anomalous Mixing Effects in f-Electron Systems, J. Magn. Magn. Mater. **52**, 145 (1985).
80. O. Gunnarsson and K. Schönhammer: The Dynamic Susceptibility of Ce Compounds in the $1/N_f$ expansion. J. Magn. Magn. Mater. **52**, 227 (1985).
81. D.D. Sarma, F.U. Hillebrecht, O. Gunnarsson and K. Schönhammer: Systematics in the Core Level Spectra of Th-Intermetallics. Z. Phys. **B63**, 305 (1986).
82. M.J. Puska, O. Jepsen, O. Gunnarsson and R.M. Nieminen: Electronic Structure and Positron States at Vacancies in Si and GaAs. Phys. Rev. **B34**, 2695 (1986).
83. O. Gunnarsson and K. Schönhammer: Density Functional Treatment of an Exactly Solvable Semiconductor Model. Phys. Rev. Lett. **56**, 1968 (1986).
84. O. Gunnarsson and K. Schönhammer: Many-Body Theory for Spectroscopies of Ce Mixed Valence Compounds. Invited talk at 4th Int. Conference of EXAFS and Near Edge Structure. J. de Physique **C8**, 923 (1986).
85. J.W. Allen, S.-J. Oh, O. Gunnarsson, K. Schönhammer, M.B. Maple and M.S. Torikachvili: Electronic Structure of Ce and Light Rare Earths Intermetallics. Adv. Physics **35**, 275 (1986).

86. T.C. Li, O. Gunnarsson, K. Schönhammer and G. Zwicknagl: Local Fermi Liquid Theory of the Anderson Impurity Model. *J. Phys C* **20**, 405 (1987).
87. K. Schönhammer and O. Gunnarsson: Many-Body Theory for Intermediate Valence Spectroscopies. Invited talk at the Int. Conference on Anomalous Rare Earths and Actinides, *J. Magn. Mater.* **63-64**, 481 (1987).
88. O. Gunnarsson and K. Schönhammer: Intermediate Valence Spectroscopies. Invited Lecture at the NATO Advanced Study Institute *Giant Resonances in Atoms, Molecules and Solids*, edited by J.P. Connerade, J.M. Esteve and R.C. Karanatek (Plenum, New York, 1987) p. 405.
89. O. Gunnarsson, R.O. Jones and K. Schönhammer: Density-Functional Formalism: V_{xc} , Discontinuities and the Local Density Approximation in *Electronic Band Structure and its Application*, Lecture Notes Vol. 283, edited by M. Yussouff (Springer, Heidelberg, 1987) p. 77. Invited talk at the international school on Electronic Band Structure and its Applications, Kanpur, India, 1986.
90. K. Schönhammer and O. Gunnarsson: Discontinuity of the Exchange-Correlation Potential in Density Functional Theory. *J. Phys. C* **20**, 3675 (1987).
91. F. Beeler, O.K. Andersen, O. Gunnarsson, O. Jepsen and M. Scheffler: Electronic-Structure Calculation of Point Defects in Silicon. Invited Paper at the Symposium of Computational Physics (Amsterdam, 1986), *Computer Phys. Commun.* **44**, 297 (1987).
92. O. Gunnarsson and T.C. Li: Resonance Photoemission for f-electron Systems. *Phys. Rev.* **B36**, 9488 (1987).
93. O. Gunnarsson and K. Schönhammer: Many-Body Theory for Spectra of f-electron Systems. *Physica Scripta* **T19**, 273 (1987). Invited talk at the 7th General Conference of the Condensed Matter Division-EPS, Pisa, 1987.

94. O. Gunnarsson and K. Schönhammer: Many-Body Formulation of Spectra of Mixed Valence Systems in *Handbook on the Physics and Chemistry of Rare Earths* edited by K.A. Gschneider, L. Eyring and S. Hufner (North-Holland, Amsterdam, 1987), Vol. 10, p. 103.
95. K. Schönhammer, L. Bönig and O. Gunnarsson: Electron Friction in Metals and at Metal Surfaces. *Prog. Surf. Sci.* **26**, 1 (1987).
96. J.C. Fuggle, O. Gunnarsson, G.A. Sawatzky and K. Schönhammer: Virtual-bound-state effects in core-level spectra of light rare-earth alloys. *Phys. Rev. B* **37**, 1103 (1988).
97. S.-J. Oh, S. Suga, A. Kakizaki, M. Taniguchi, T. Ishii, J.-S. Kang, J. W. Allen, O. Gunnarsson, N. Christensen, A. Fujimori, T. Suzuki, T. Kasuya, T. Miyahara, H. Kato, K. Schönhammer, M. S. Torikachvili and M. B. Maple: Observation of Kondo resonance in YbAl₃. *Phys. Rev. B* **37**, 2861 (1988).
98. O. Gunnarsson, D.D. Sarma, F.U. Hillebrecht and K. Schönhammer: Electronic Structure of the light Actinide Oxides from Electron Spectroscopy. Invited talk at the 32nd annual conf. on magnetism and magnetic materials, 1987. *J. Appl. Phys.* **63**, 3676 (1988).
99. K. Schönhammer and O. Gunnarsson: Model Hamiltonians and how to determine their parameters. Invited talk at the NATO Workshop Narrow-Band Phenomena - Influence of Electrons with both Band and Localized Character, edited by J.C. Fuggle, G.A. Sawatzky and J.W. Allen (Plenum, New York, 1988), p. 127.
100. K. Schönhammer and O. Gunnarsson: Difference between the Quasiparticle and Kohn-Sham-Fermi Surfaces. *Phys. Rev B (Rapid Commun.)* **37**, 3128 (1988).
101. A. Svane and O. Gunnarsson: Localization in the self-interaction-corrected density-functional formalism. *Phys. Rev. B (Rapid Commun.)* **37**, 9919 (1988).

102. O. Gunnarsson, O.K. Andersen, O. Jepsen and J. Zaanen. Ab Initio Calculation of the Parameters in the Anderson model. Invited talk at the 10th Tanigushi Symposium *Core level Spectroscopy in condensed systems*, edited by J. Kanamori and A. Kotani, (Springer, Berlin, 1988), p. 82.
103. J. Zaanen, O. Jepsen, O. Gunnarsson, A.T. Paxton, O.K. Andersen and A. Svane: What can be learned about high T_c from local density theory? *Physica C* **153-155**, 1636 (1988).
104. A. Svane and O. Gunnarsson: Anti-Ferromagnetic Moment Formation in the Self-Interaction Corrected Density Functional Formalism. *Europhys. Lett.* **7**, 171 (1988).
105. O. Gunnarsson and O. Jepsen: Configuration Dependence of hopping matrix elements in the Anderson model. *Phys. Rev. B* **38**, 3568 (1988).
106. N.E. Christensen, O. Gunnarsson, O. Jepsen and O.K. Andersen: Local spin density theory for ferro- and antiferromagnetic materials. Invited talk at the international conference on magnetism, Paris, France, July 25-29, 1988. *J. de Physique* **C8**, 17 (1988).
107. N.E. Christensen, O.K. Andersen, O. Gunnarsson and O. Jepsen: Density Functional Calculations of Fermi Surfaces of Normal and Heavy-Electron Metals. Invited talk at the 6th Inter. Conf. on Crystal-Field Effects and Heavy-Fermion Physics. *J. Magn. Mater.* **76&77**, 23 (1988).
108. O. Gunnarsson, N.E. Christensen and O.K. Andersen: Density Functional Calculations for $4f$ -Electron Systems: Hopping Matrix Elements for the Anderson Model. Invited talk at the 6th Inter. Conf. on Crystal-Field Effects and Heavy-Fermion Physics. *J. Magn. Mater.* **76 & 77**, 30 (1988).
109. O. Gunnarsson, O.K. Andersen, O. Jepsen and J. Zaanen: Density-functional calculation of the parameters in the Anderson model: Application to Mn in CdTe. *Phys.*

- Rev. B **39**, 1708 (1989).
110. A. Svane and O. Gunnarsson: Localization in the self-interaction-corrected density functional formalism. *J. de Chemie Physique* **86**, 823 (1989).
 111. R.O. Jones and O. Gunnarsson: The density functional formalism, its applications and prospects. *Rev. Mod. Phys.* **61**, 689 (1989).
 112. P. Bagno, O. Jepsen, O. Gunnarsson: Ground-state properties of third-row elements with nonlocal density functionals. *Phys. Rev. B (Rapid Commun.)* **40**, 1997 (1989).
 113. J. Zaanen and O. Gunnarsson: Charged magnetic domain lines and the magnetism of the high- T_c oxides. *Phys. Rev. B (Rapid Commun.)* **40**, 7391 (1989).
 114. O. Gunnarsson, O.K. Andersen and A. Svane: Density Functional Calculations for Strongly Correlated Systems, Invited talk at the NATO workshop *Interacting Electrons in Reduced Dimensions*, Torino 1988, edited by D. Baeriswyl and D.K. Campbell, (Plenum, New York, 1989), NATO Advanced Research Workshop, Vol. 213, p. 139.
 115. O. Gunnarsson, A.V. Postnikov and O.K. Andersen: Density- functional calculation of Coulomb interaction strengths in nonmetallic systems: Applications to Mn in CdTe, CdS and ZnO. *Phys. Rev. B* **40**, 10407 (1989).
 116. O. Gunnarsson and K. Schönhammer: Renormalization of hopping integrals due to Coulomb interactions for the Anderson model. *Phys. Rev. B* **40**, 4160 (1989).
 117. G.P. Das, P. Blöchl, O.K. Andersen, N.E. Christensen, and O. Gunnarsson: Electronic structure and Schottky-barrier heights of (111) NiSi₂/Si A- and B- type Interfaces. *Phys. Rev. Lett.* **63**, 1168 (1989).
 118. O. Gunnarsson, P. Gies, W. Hanke and O.K. Andersen: *Ab initio* method for calculating response functions in transition metals. *Phys. Rev. B* **40**, 12140 (1989).

119. J. Zaanen and O. Gunnarsson: Local spin screening in the High T_c superconductors. *Physica C* **162-164**, 821 (1989).
120. O. Gunnarsson: Probes of hybridization and Coulomb correlation in valence states using ab initio calculations and high energy spectroscopies. Plenary talk at the 2nd European Conference on Progress in X-Ray Synchrotron Radiation Research, edited by A. Balerna, E. Bernieri and S. Mobilio (Societa Italiana di Fisica, Bologna, 1990) Conference Proceedings Vol. 25, p. 77.
121. A. Svane and O. Gunnarsson: Transition-metal oxides in the self-interaction corrected density functional formalism. *Phys. Rev. Lett.* **65**, 1148 (1990).
122. O. Gunnarsson: Calculation of parameters in model Hamiltonians. *Phys. Rev. B* **41**, 514 (1990).
123. A. Svane and O. Gunnarsson: Hydrogen solid in self-interaction-corrected local-spin-density approximation. *Solid State Commun.* **76**, 851 (1990).
124. O. Gunnarsson, J.W. Allen, O. Jepsen, T. Fujiwara, O.K. Andersen, C.G. Olsen, M.B. Maple, J.-S. Kang, L.Z. Liu, J.-H. Park, R.O. Anderson, W.P. Ellis, R. Liu, J.T. Markert, Y. Dalichaouch, Z.-X. Shen, P.A.P. Lindberg, B.O. Wells, D.S. Dessau, A. Borg, I. Lindau, and W.E. Spicer: Polarized resonance photoemission for Nd_2CuO_4 . *Phys. Rev. B (Rapid Commun.)* **41**, 4811 (1990).
125. O. Gunnarsson, O. Jepsen and Z.-X. Shen: Local singlet for CuO and Nd_2CuO_4 . *Phys. Rev. B (Rapid Commun.)* **42**, 8707 (1990).
126. J.W. Allen, J.-S. Kang, L.-Z. Liu, O. Gunnarsson, N.E. Christensen, O.K. Andersen, M.B. Mapl, M.S. Torikachvili, D.D. Koelling, W.P. Ellis, B.B. Pate, Z.-X. Shen, J.J. Yeh and I. Lindau: Electron spectroscopy of heavy-Fermion materials. Invited talk at the 9th International Conference on Vacuum Ultraviolet Radiation Physics, Honolulu, Hawaii, July 17-21, 1989, *Physica Scripta* **T31**, 232 (1990).

127. J.-S. Kang, J.W. Allen, O. Gunnarsson, N.E. Christensen, O.K. Andersen, Y. Lassailly, M.B. Maple, and M.S. Torikachvili: Origin of heavy-fermion behaviour in CeCu_2Si_2 . *Phys. Rev. B* **41**, 6610 (1990).
128. G.P. Das, P. Blöchl, O.K. Andersen, N.E. Christensen, and O. Gunnarsson: Das et al. Reply. *Phys. Rev. Lett.* **65**, 2084 (1990).
129. V.I. Anisimov and O. Gunnarsson: Density-functional calculation of effective Coulomb interactions in metals. *Phys. Rev. B* **43**, 7570 (1991).
130. V. Drchal, O. Gunnarsson and O. Jepsen: Effective Coulomb interaction in metallic $3d$ system: Comparison of theory and experiment for Mn in Ag. *Phys. Rev. B* **44**, 3518 (1991).
131. K. Schönhammer, I. Stübiger and O. Gunnarsson: Resonant excitation of electron-hole pairs in semiconductors: A simplified model. *Phys. Rev. B* **44**, 7965 (1991).
132. L. Braicovich, C. Carbone, O. Gunnarsson, and G.L. Olcese: Resonant photoemission from $\text{Ce}_{24}\text{Co}_{11}$ at the $4d$ - $4f$ threshold. *Phys. Rev. B* **44**, 13756 (1991).
133. O. Gunnarsson: Transition metal oxides in the self-interaction-corrected density functional formalism. Invited talk at the American Physical Society March meeting, Cincinnati, 1991, *Bull. Am. Phys. Soc.* **36**, 533 (1991).
134. O.K. Andersen, A.I. Liechtenstein, O. Rodriguez, I.I. Mazin, O. Jepsen, V.P. Antropov, and O. Gunnarsson: Electrons, phonons, and their interactions in $\text{YBa}_2\text{Cu}_3\text{O}_7$. Invited talk at the International Conference on materials and mechanisms of Superconductivity - High temperature superconductivity, Kanazawa, Japan, July 22-26, 1991. *Physica C* **185-189**, 147 (1991).
135. O. Gunnarsson, S. Satpathy, O. Jepsen, and O.K. Andersen: Orientation of C_{60} clusters in solids. *Phys. Rev. Lett.* **67**, 3002 (1991).

136. K. Karlsson, O. Gunnarsson and O. Jepsen: Chemical shifts for monovalent, divalent and trivalent Cu compounds. *J. Phys.: Condens. Matter* **4**, 895 (1992).
137. K. Karlsson, O. Gunnarsson and O. Jepsen: Shape of the Cu $2p$ core level photoemission spectrum for monovalent, divalent and trivalent Cu compounds. *J. Phys.: Condensed Matter* **4**, 2801 (1992).
138. L.Z. Liu, J.W. Allen, O. Gunnarsson, N.E. Christensen, and O.K. Andersen: $\alpha - \gamma$ transition in Ce: A detailed analysis of electron spectroscopy. *Phys. Rev. B* **45**, 8934 (1992).
139. S. Satpathy, V.P. Antropov, O.K. Andersen, O. Jepsen, O. Gunnarsson, and A.I. Liechtenstein: Conduction-band structure of alkali-metal-doped C_{60} . *Phys. Rev. B* **46**, 1773 (1992).
140. S.-J. Oh, J.-S. Kang, J.W. Allen, S. Suga, A. Kakizaki, M. Taniguchi, T. Ishii, O. Gunnarsson, N.E. Christensen, A. Fujimori, T. Suzuki, T. Kasuya, T. Miyahara, H. Kato, K. Schönhammer, M. S. Torikachvili and M. P. Maple: Reply to "Comment on 'Observation of Kondo resonance in $YbAl_3$ ' ". *Phys. Rev. B* **46**, 1866 (1992).
141. O. Gunnarsson: Model Hamiltonian parameters from *ab initio* calculations. Invited talk at the 2nd ISSP International Symposium on Physics and Chemistry of Oxide Superconductors, Tokyo, January 16-18, 1991 (Editors Y. Iye and H. Yasuoka, Springer, Berlin, 1992) p. 95.
142. O. Gunnarsson: Resonance photoemission in strongly correlated systems. Invited talk at the 2nd international workshop on Auger Spectroscopy and Electronic Structure, Malmö, 4-6 Sept. 1991, *Physica Scripta* **T41**, 12 (1992).
143. O. Gunnarsson, K. Karlsson, and O. Jepsen: Chemical shifts and line shapes for monovalent, divalent and trivalent Cu compounds, invited talk at the 48th international meeting on Synchrotron radiation and dynamic phenomena, Grenoble 9-13 Sept. 1991,

- American Institute of Physics Conference Proceedings no. 258, Editor A. Beswick, p. 550 (1992).
144. K. Karlsson, O. Gunnarsson and O. Jepsen: Cu $2p$ chemical shifts for $\text{YBa}_2\text{Cu}_3\text{O}_{6.5}$: Valence of the Cu atoms. *Phys. Rev. B (Rapid Commun.)* **45**, 7559 (1992).
 145. S. Gopalan, O. Gunnarsson and O.K. Andersen: Effects of saddle-point Singularities on the electron life-time. *Phys. Rev. B* **46**, 11798 (1992).
 146. V.P. Antropov, O. Gunnarsson, and O. Jepsen: Coulomb integrals and model Hamiltonians for C_{60} . *Phys. Rev. B (Rapid Commun.)* **46**, 13647 (1992).
 147. L. Braicovich, F. Ciccacci, E. Puppini, A. Svane, and O. Gunnarsson: Ultraviolet inverse photoemission from iron monoxide and self-interaction-corrected local-spin-density calculations. *Phys. Rev. B* **46**, 12165 (1992).
 148. O. Gunnarsson and G. Zwicknagl: Coulomb pseudopotential, screening and superconductivity in C_{60} . *Phys. Rev. Lett.* **69**, 957 (1992).
 149. O. Gunnarsson and J. Zaanen: Impurity-spin screening in low-density Fermi liquids. *Phys. Rev. B* **46**, 15019 (1992).
 150. O. Gunnarsson, D. Rainer and G. Zwicknagl: Screened interaction and Coulomb pseudo-potential in C_{60} , Invited talk at the Adriatico Research Conference on “Clusters and Fullerenes” 23-26 June 1992 in Trieste, *Int. J. Mod. Phys. B* **6**, 3993 (1992).
 151. M. Knupfer, M. Merkel, M.S. Golden, J. Fink, O. Gunnarsson, and V.P. Antropov: Satellites in the photoemission spectra of A_3C_{60} ($\text{A}=\text{Rb}$ and K). *Phys. Rev. B (Rapid Commun.)* **47**, 13944 (1993).
 152. V.P. Antropov, O. Gunnarsson, and A.I. Liechtenstein: Phonons, electron-phonon and electron-plasmon coupling in C_{60} compounds: *Phys. Rev. B* **48**, 7651 (1993).

153. P.A. Brühwiler, A.J. Maxwell, A. Nilsson, N. Mårtensson, and O. Gunnarsson: Auger and photoelectron study of the Hubbard U in C_{60} , K_3C_{60} and K_6C_{60} . *Phys. Rev. B* **48**, 18296 (1993).
154. M. Knupfer, M. Merkel, M.S. Golden, J. Fink, O. Gunnarsson, and V.P. Antropov: High resolution photoemission studies of A_3C_{60} ($A=Rb, K$). Invited talk at the International Winterschool on Electronic Properties of Fullerenes, Kirchberg, Austria, 6-13 March, 1993, *Electronic Properties of Fullerenes*, Eds. H. Kuzmany, J. Fink, M. Mehring, and S. Roth, Springer Series in Solid State Sciences 117, Springer, Berlin, 1993, p. 114.
155. I.I. Mazin, A.I. Liechtenstein, O. Gunnarsson, O.K. Andersen, V.P. Antropov, and S.E. Burkov: Orientational order in A_3C_{60} : Antiferromagnetic Ising model for the fcc lattice, *Phys. Rev. Lett.* **70**, 4142 (1993).
156. A.I. Liechtenstein, I.I. Mazin, O. Gunnarsson, O.K. Andersen, S.E. Burkov, and V.P. Antropov: Orientational order in A_3C_{60} : Effects on valence bands and infrared optical spectra. Invited talk at the International Winterschool on Electronic Properties of Fullerenes, Kirchberg, Austria, 6-13 March, 1993, *Electronic Properties of Fullerenes*, Eds. H. Kuzmany, J. Fink, M. Mehring, and S. Roth, Springer Series in Solid State Sciences 117, Springer, Berlin, 1993, p. 211.
157. J.W. Allen and O. Gunnarsson: Crucial but Overlooked Aspects of Photoemission in small T_K Cerium Materials, *Phys. Rev. Lett.* **70**, 1180 (1993).
158. O. Gunnarsson, V.P. Antropov, J. Fink, M.S. Golden, M. Knupfer, A.I. Liechtenstein, M. Merkel, D. Rainer and G. Zwicknagl: "Electron-phonon coupling, Coulomb pseudopotential μ^* and physical properties of doped C_{60} compounds" Invited talk at the NATO Advanced Research Workshop on "Physics and Chemistry of the Fullerenes", 7-13.6.1993, Aghia Pelaghia, Crete, Greece, NATO ASI series C: Mathematical and Physical Sciences-Vol. 443, Ed. K. Prassides, Kluwer, Dordrecht, 1994, p. 263.

159. O. Jepsen, K. Karlsson and O. Gunnarsson: Electronic structure and photoemission spectra of Cu compounds, Invited talk at the 9th Int. Conference on ternary and multinary compounds, Yokohama, Japan, 8-12.8.1993, Jap. J. Appl. Phys. **32** Suppl. 32-3, 212 (1994).
160. F. Aryasetiawan and O. Gunnarsson: Linear muffin-tin orbital method with multiple orbitals per L channel. Phys. Rev. B **49**, 7219 (1994).
161. F. Aryasetiawan and O. Gunnarsson: Product-basis method for calculating dielectric matrices. Phys. Rev. B **49**, 16214 (1994).
162. F. Aryasetiawan, O. Gunnarsson, M. Knupfer, J. Fink: Local-field effects in NiO and Ni. Phys. Rev. B **50**, 7311 (1994).
163. I.I. Mazin, A.I. Liechtenstein, O. Gunnarsson and O.K. Andersen: Three-molecular-orbital treatment of the orientational ordering in A_3C_{60} . Solid State Commun. **91**, 497 (1994).
164. O. Gunnarsson, V. Meden and K. Schönhammer: Corrections to Migdal's theorem for spectral functions: A cumulant treatment of the time-dependent Green's function. Phys. Rev. B **50**, 10462 (1994).
165. O. Gunnarsson, K. Schönhammer and V. Meden: Corrections to Migdal's theorem for photoemission spectra. Invited talk at the International Winterschool on Electronic Properties of Novel Materials, Kirchberg, Austria, 5-12 March, 1994, *Progress in Fullerene Research*, Eds. H. Kuzmany, J. Fink, M. Mehring, and S. Roth, World Scientific, Singapore, 1994, p. 317.
166. V. Meden, K. Schönhammer and O. Gunnarsson: Electron-phonon interaction in one dimension: Exact spectral properties. Phys. Rev. B **50**, 11179 (1994).
167. O. Gunnarsson, H. Handschuh, P.S. Bechthold, B. Kessler, G. Ganteför, and W. Eberhardt: Photoemission Spectra of C_{60}^- ; Electron-Phonon coupling, Jahn-Teller effect

- and Superconductivity in the Fullerenes. Phys. Rev. Lett. **74**, 1875 (1995).
168. O. Gunnarsson, Jahn-Teller effect and on-site interaction for C_{60}^{n-} . Phys. Rev. B **51**, 3493 (1995).
169. O. Gunnarsson, Electron-phonon interaction and physical properties of doped fullerenes. Invited talk at the APS March meeting 1995, Bull. Am Phys. Soc. **40**, 150 (1995).
170. F. Aryasetiawan and O. Gunnarsson: The electronic structure of NiO in the GW approximation. Phys. Rev. Lett. **74**, 3221 (1995).
171. N. Laouini, O.K. Andersen, O. Gunnarsson: Analytical Molecular Orbitals and Band Structures of solid C_{60} . Phys. Rev. B **51**, 17446 (1995).
172. G. Ganteför, C.-Y. Cha, H. Handschuh, G. Schulze Icking-Konert, B. Kessler, O. Gunnarsson, and W. Eberhardt: Electronic and geometric structure of small mass selected clusters. J. Elec. Spect. Rel. Phenom. **76**, 37 (1995).
173. O. Gunnarsson, A.I. Liechtenstein, V. Eyert, M. Knupfer, J. Fink, Armbruster: Plasmon damping and dispersion in doped C_{60} compounds. Invited talk at the International Winterschool on Electronic Properties of novel Materials, Kirchberg, Austria, 4-10 March, 1995, *Physics and Chemistry of Fullerenes and Derivatives*, Eds. H. Kuzmany, J. Fink, M. Mehring, and S. Roth, World Scientific, 1995, p. 402.
174. K. Schönhammer, O. Gunnarsson and R.M. Noack: Density functional theory on a lattice: Comparison with exact numerical results for a model with strongly correlated electrons. Phys. Rev. B **52**, 2504 (1995).
175. O. Gunnarsson, A.I. Liechtenstein, V. Eyert, M. Knupfer, J. Fink, J.F. Armbruster: Plasmon dispersion and broadening in A_3C_{60} (A=K, Rb). Phys. Rev. B **53**, 3455 (1996).

176. E. Koch and O. Gunnarsson: Density dependence of the electronic supershells in the homogeneous jellium model. *Phys. Rev. B* **54**, 5168 (1996).
177. O. Gunnarsson, V. Eyert, M. Knupfer, J. Fink, J.F. Armbruster: Plasmon dispersion in A_3C_{60} ($A=K, Rb$). *J. Phys.: Cond. Matter* **8**, 2557 (1996).
178. E. Tosatti, N. Manini and O. Gunnarsson: Surprises in the orbital magnetic moment and g factor of the dynamic Jahn-Teller ion C_{60}^- . *Phys. Rev. B* **54**, 17184 (1996).
179. A.I. Liechtenstein, O.Gunnarsson, M. Knupfer, J. Fink, J.F. Armbruster: Plasmon damping and response function in doped C_{60} compounds. *J. Phys.: Cond. Matter* **8**, 4001 (1996).
180. F. Aryasetiawan and O. Gunnarsson: 3d semicore states in ZnSe, GaAs and Ge, *Phys. Rev. B* **54**, 17564 (1996).
181. O. Gunnarsson: Local-field effects and quasi-particle band structure in localized systems, Invited talk at the APS March meeting 1996, *Bull. Am Phys. Soc.* **41**, 495 (1996).
182. O. Gunnarsson, E. Koch, R.M. Martin: Mott transition in degenerate Hubbard models: Application to doped fullerenes, *Phys. Rev. B* **54**, R11026 (1996).
183. A.I. Liechtenstein, O. Gunnarsson, R.M. Martin, and O.K. Andersen: Quasiparticle bands and superconductivity in bilayer cuprates, *Phys. Rev. B* **54**, 12505 (1996).
184. S.K. Mishra, S. Satpathy, F. Aryasetiawan, and O. Gunnarsson: Possible suppression of canted spin order in the double-exchange lanthanum manganites, *Phys. Rev. B* **55**, 2725 (1997).
185. O. Gunnarsson: Superconductivity in Fullerides, *Rev. Mod. Phys.* **69**, 575 (1997).

186. P. Ziesche, O. Gunnarsson, W. John, and H. Beck: Two-site Hubbard model and BCS model - naturally analyzed and the concept of correlation entropy, *Phys. Rev. B* **55**, 10270 (1997).
187. F. Aryasetiawan, O. Gunnarsson, E. Koch, and R.M. Martin: Pauli susceptibility of A_3C_{60} ($A= K, Rb$), *Phys. Rev. B* **55**, R10165 (1997).
188. O. Gunnarsson, E. Koch, R.M. Martin: Mott-Hubbard insulators for systems with orbital degeneracy, *Phys. Rev. B* **56**, 1146 (1997).
189. O. Gunnarsson: Electron self-energy in A_3C_{60} ($A=K, Rb$): Effects of t_{1u} plasmon in GW approximation, *J. Phys.: Cond. Matt.* **9**, 5635 (1997).
190. O. Gunnarsson: Hubbard model with orbital degeneracy and integer or noninteger filling. *Z. Phys. B* **104**, 279 (1997).
191. O. Gunnarsson and E. Koch: Discrete Hubbard-Stratonovich transformation for systems with orbital degeneracy, *Phys. Lett. A* **235**, 530 (1997).
192. O. Gunnarsson, E. Koch, R.M. Martin, and F. Aryasetiawan: Metallicity, susceptibility and superconductivity in A_3C_{60} ($A= K, Rb$), invited talk at the 191st Electrochemical Society meeting, Montreal, May 4-9, 1997, *Recent Advances in the Chemistry and Physics of Fullerenes and related Materials* Vol. 4, Eds. K.M. Kadish and R.S. Ruoff, Electrochemistry Society Proceedings 97-14, page 1040 (1997).
193. O. Gunnarsson: Effects of nonstoichiometry in $A_{3-x}C_{60}$ ($A= K, Rb$), invited talk at the 192nd Electrochemical Society meeting, Paris, Sept. 1-5, 1997, *Recent Advances in the Chemistry and Physics of Fullerenes and related Materials* Vol. 5, Eds. K.M. Kadish and R.S. Ruoff, Electrochemistry Society Proceedings 97-42, page 488 (1997).
194. O. Gunnarsson, S.C. Erwin, E. Koch, and R.M. Martin: Role of alkali atoms in A_4C_{60} , *Phys. Rev. B* **57**, 2159 (1998).

195. J. van den Brink, O. Gunnarsson, and V. Eyert: Optical conductivity in A_3C_{60} ($A=K, Rb$), Phys. Rev. B **57**, 2163 (1998).
196. O. Gunnarsson, E. Koch, R.M. Martin, and F. Aryasetiawan: Correlation effects in doped C_{60} compounds, Invited talk at the International Winterschool on Electronic Properties of novel Materials, Kirchberg, Austria, 1-8 March, 1997, *Molecular Nanostructures*, Eds. H. Kuzmany, J. Fink, M. Mehring, and S. Roth, World Scientific, 1998, p. 229.
197. E. Koch, O. Gunnarsson, and R.M. Martin: Quantum Monte-Carlo calculations for integer-doped fullerides, International Winterschool on Electronic Properties of novel Materials, Kirchberg, Austria, 1-8 March, 1997, *Molecular Nanostructures*, Eds. H. Kuzmany, J. Fink, M. Mehring, and S. Roth, World Scientific, 1998, p. 235.
198. O. Gunnarsson, E. Koch and R.M. Martin: Superconductivity in doped C_{60} compounds, Invited talk in the International School of solid state physics, Erice, June 4-11, 1997, "Pair Correlation in Many-Fermion Systems", Ed. V. Z. Kresin, Plenum (New York, 1998) p. 155.
199. F. Aryasetiawan and O. Gunnarsson: The GW method, Rep. Prog. Phys. **61**, 237 (1998).
200. O. Gunnarsson: Electron correlation in doped fullerides, Invited talk at the APS March meeting 16-20.3.1998. Bull. Am. Phys. Soc. **43**, 353 (1998).
201. O. Gunnarsson, E. Koch, and R.M. Martin: Mott transition and superconductivity in alkali-doped fullerides, Invited talk at the International Winterschool on Electronic Properties of novel Materials, Kirchberg, Austria, 28.02-07.03.1998, , Eds. H. Kuzmany, J. Fink, M. Mehring, and S. Roth, AIP Conference Proceedings 442, (Woodbury, New York, 1998), p. 287.

202. E. Koch, O. Gunnarsson, and R.M. Martin: Dielectric screening in doped Fullerenes, International Winterschool on Electronic Properties of novel Materials, Kirchberg, Austria, 28.02-07.03.1998, , Eds. H. Kuzmany, J. Fink, M. Mehring, and S. Roth, AIP Conference Proceedings 442, (Woodbury, New York, 1998), p. 292.
203. K. Karlsson, O. Gunnarsson, and O. Jepsen: Cuprate core level line shapes for different Cu-O networks, *Phys. Rev. Lett.* **82**, 3528 (1999).
204. E. Koch, O. Gunnarsson and R.M. Martin: Fixed-node DMC for Fermions on a lattice: Application to the doped Fullerenes, *Quantum Monte Carlo Methods in Physics and Chemistry*, Proceedings of the NATO-ASI, Eds.: M.P. Nightingale and C.J. Umrigar (Kluwer Academic Publishers, 1999), p447.
205. J.E. Han, O. Gunnarsson, and V. Eyert: Phonon line shape in disordered A_3C_{60} ($A=K, Rb$), *Phys. Rev. B* **60**, 6495 (1999).
206. E. Koch, O. Gunnarsson and R.M. Martin: Screening, Coulomb pseudopotential and superconductivity in alkali-doped Fullerenes, *Phys. Rev. Lett.* **83**, 620 (1999).
207. E. Koch, O. Gunnarsson, and R.M. Martin: Optimization of Gutzwiller wave-functions in quantum Monte-Carlo, *Phys. Rev. B* **59**, 15632 (1999).
208. J.D. Lee, O. Gunnarsson and L. Hedin, Transition from the adiabatic to the sudden limit in photoemission: A model study of a localized system, *Phys. Rev. B* **60**, 8034 (1999).
209. J.E. Han and O. Gunnarsson: Phonon spectral function for an interacting electron-phonon system, *Phys. Rev. B* **61**, 8628 (2000).
210. K. Schönhammer, V. Meden, W. Metzner, U. Schollwöck, and O. Gunnarsson: Boundary effects on photoemission spectra of Luttinger liquids, *Phys. Rev. B* **61**, 4393 (2000).

211. E. Koch, O. Gunnarsson and R.M. Martin: Screening of a point charge: A fixed-node diffusion Monte Carlo study, *Computer Simulation Studies in Condensed Matter Physics XII*, Eds.: D.P. Landau, S.P. Lewis, and H.B. Schttler (Springer Verlag, Heidelberg, 1999)
212. E. Koch, O. Gunnarsson and R.M. Martin: Metal-Insulator transitions in generalized Hubbard models, Proceedings of the CCP99/Centennial Conference of the APS, *Computer Physics Communications* **127**, 137 (2000).
213. E. Koch and O. Gunnarsson: One-electron bands, quantum Monte Carlo, and real superconductors, Proceedings of the International Conference on Statistical Mechanics and Strongly Correlated Systems, *Physica A* **280**, 166 (2000).
214. E. Koch, O. Gunnarsson, and R.M. Martin: Filling dependence of the Mott transition in the degenerate Hubbard model, *Phys. Rev. B* **60**, 15714 (1999).
215. O. Gunnarsson and J.E. Han: Raman line shapes in A_3C_{60} : Effects of orientational disorder on phonon spectra, invited talk at the 195th meeting of the Electrochemical Society in Seattle, 2-6.05.99. *Recent Advances in the Chemistry and Physics of Fullerenes and related Materials* Vol. , Eds. P.V. Kamat, D.M. Guldi, K.M. Kadish, Electrochemistry Society Proceedings Vol. 99-12, page 588-596 (1999).
216. J.E. Han and O. Gunnarsson: Metal-insulator transition in systems with electron-phonon and Coulomb interactions, *Physica B* **292**, 196 (2000).
217. J.E. Han, E. Koch, and O. Gunnarsson: Metal-insulator transitions: Influence of lattice structure, Jahn-Teller effect, and Hund's rule coupling, *Phys. Rev. Lett.* **84**, 1276 (2000).
218. J.W. Allen, G.-H. Gweon, H.T. Schek, L.-Z. Liu, L.H. Tjeng, J.-H. Park, W.P. Ellis, C.T. Chen, O. Gunnarsson, O. Jepsen, O.K. Andersen, Y. Dalichaouch, M.B. Maple:

- Kondo resonance behaviour of heavy fermion f-electron materials, *J. Appl. Phys.* **87**, 6088 (2000).
219. O. Gunnarsson and J.E. Han: The mean free path for electron conduction in metallic fullerenes. *Nature* **405**, 1027 (2000).
220. O. Gunnarsson and J.E. Han: Resistivity of metallic A_3C_{60} ($A=K, Rb$): No lower limit to the mean free path? Invited talk at the International Winterschool on Electronic Properties of novel Materials - Molecular Nanostructures, Kirchberg, Austria, 4.03-11.03.2000, , Eds. H. Kuzmany, J. Fink, M. Mehring, and S. Roth, AIP Conference Proceedings 544, (Melville, New York, 2000), p. 9.
221. K. Karlsson, O. Gunnarsson, and O. Jepsen: Core level chemical shifts and lines shapes for systems with different valencies and Cu-O networks, *Int. J. Mod. Phys. B* **14**, 3791 (2000).
222. O. Gunnarsson: C_{60} : The hole story, *Nature* **408**, 528 (2000).
223. O. Gunnarsson, K. Schönhammer, J.W. Allen, K. Karlsson, and O. Jepsen: Information from photoemission spectral weights and shapes, *J. El. Spect. Rel. Phenom.* **117-118**, 1 (2001).
224. O. Gunnarsson and J.E. Han: Electron-phonon coupling in A_3C_{60} ($A=K, Rb$), Invited talk at the International Winterschool on Electronic Properties of novel Materials - Molecular Nanostructures, Kirchberg, Austria, 3.03-10.03.2001, , Eds. H. Kuzmany, J. Fink, M. Mehring, and S. Roth, AIP Conference Proceedings 591, (Melville, New York, 2001), p. 425.
225. O. Gunnarsson: "Electrical resistivity: Can the mean-free path be shorter than the lattice parameter?", invited talk at the APS March meeting, Seattle, 12-16.03.01, *Bull. Am. Phys. Soc.* **46**, 483 (2001).

226. M. Calandra and O. Gunnarsson: Saturation of electrical resistivity in metals at large temperatures, *Phys. Rev. Lett.* **87**, 266601 (2001).
227. F. Aryasetiawan, O. Gunnarsson, and A. Rubio: Excitation energies from time-dependent density-functional formalism for small systems. *Europhys. Lett.* **57**, 683 (2002).
228. R.E. Dinnebier, O. Gunnarsson, H. Brumm, E. Koch, P.W. Stephens, A. Huq, and M. Jansen: Structure of haloform intercalated C_{60} and its influence on superconductive properties. *Science* **296**, 109 (2002).
229. A. Koitzsch, J. Fink, M.S. Golden, K. Karlsson, O. Jepsen, and O. Gunnarsson, L.L. Miller, H. Eisaki, S. Uchida, G. Yang, and S. Abell: Core hole screening response in two-dimensional cuprates: A high-resolution x-ray photoemission study, *Phys. Rev. B* **66**, 024519 (2002)
230. F. Aryasetiawan and O. Gunnarsson: Exchange-correlation kernel in time-dependent density theory. *Phys. Rev. B* **66**, 165119 (2002).
231. M. Calandra and O. Gunnarsson: Electrical resistivity at large temperatures: Saturation and lack thereof, *Phys. Rev. B.* **66**, 205105 (2002).
232. M. Calandra and O. Gunnarsson: Violation of Ioffe-Regel condition but saturation of resistivity of the high- T_c cuprates. *Europhys. Lett.* **61**, 88 (2003).
233. O. Gunnarsson and K. Schönhammer: Comment on “Bethe Ansatz Results for the $4f$ -Electron Spectra of a Degenerate Anderson Model”, *Phys. Rev. Lett.* **90**, 099701 (2003)
234. J.E. Han, O. Gunnarsson, and V.H. Crespi: Strong superconductivity with local Jahn-Teller phonons in C_{60} solids, *Phys. Rev. Lett.* **90**, 167006 (2003).

235. E. Koch and O. Gunnarsson: Possibility of coupling to haloform molecules in intercalated C_{60} , *Phys. Rev. B* **67**, 161402(R) (2003).
236. O. Gunnarsson, M. Calandra, and J.E. Han: Saturation of electrical resistivity, *Rev. Mod. Phys.* **75**, 1085 (2003).
237. S. Ahlert, W. Klein, O. Jepsen, O. Gunnarsson, O.K. Andersen, M. Jansen: $Ag_{13}OsO_6$: A silver oxide with interconnected icosahedral Ag_{13}^{+4} clusters and dispersed OsO_6^{-4} octahedra, *Angew. Chem. Int. Ed.* **42**, 4321 (2003).
238. E. Koch, O. Gunnarsson, S. Wehrli, and M. Sigrist: Field-doping of C_{60} crystals: A view from theory, *Molecular Nanostructures: XVII Int'l Winterschool/Euroconference on Electronic properties of novel materials*, Eds. H. Kuzmany, J. Fink, M. Mehring, and S. Roth, AIP, CP685 (2003), p. 66.
239. J. Merino and O. Gunnarsson: Simple model for scanning tunneling spectroscopy of noble metal surfaces with adsorbed transition metal atoms, *Phys. Rev. B* **69**, 115404 (2004).
240. O. Rösch and O. Gunnarsson: Electron-phonon interaction in the $t - J$ model, *Phys. Rev. Lett.* **92**, 146403 (2004).
241. O. Gunnarsson: Alkali-doped fullerenes: Narrow-band solids with unusual properties, World Scientific (Singapore, 2004).
242. J. Merino and O. Gunnarsson: Role of surface states in STM spectroscopy of (111) metal surfaces with Kondo absorbers, *Phys. Rev. Lett.* **93**, 156601 (2004).
243. O. Rösch and O. Gunnarsson: Electron-phonon interaction in the three-band model, *Phys. Rev. B* **70**, 224518 (2004).
244. O. Rösch and O. Gunnarsson: Apparent electron-phonon interaction in strongly correlated systems, *Phys. Rev. Lett.* **93**, 237001 (2004).

245. J.E. Han, O. Gunnarsson, and V. H. Crespi: Superconductivity in fullerenes, chapter in "Superconducting Materials" edited by A.V. Narlikar (Springer, Berlin, 2005).
246. O. Gunnarsson, J.E. Han, E. Koch, and V.H. Crespi: Superconductivity in alkali-doped fullerenes, *Structure & Bonding*, Vol. **114**, p. 71, Eds. K. A. Müller, A. Bussmann-Holder, Springer (2005).
247. O. Rösch, J. E. Han, O. Gunnarsson and V. H. Crespi: Interplay between electron-phonon and electron-electron interactions, *physica status solidi b* **242**, 118 (2005).
248. O. Rösch and O. Gunnarsson: Dispersion of incoherent spectral features in systems with strong electron-phonon coupling, *Eur. Phys. J. B* **43**, 11 (2005).
249. O. Rösch, O. Gunnarsson, X. J. Zhou, T. Yoshida, T. Sasagawa, A. Fujimori, Z. Hussain, Z.-X. Shen and S. Uchida: Polaronic behavior of undoped high- T_c cuprate superconductors from angle-resolved photoemission spectra, *Phys. Rev. Lett.* **95**, 227002 (2005).
250. O. Gunnarsson: Polaronic behavior and electron-phonon interaction in cuprates, Invited talk at the APS meeting in Los Angeles. *Bull. Am. Phys. Soc.* **46** (2005).
251. O. Gunnarsson and O. Rösch: Electron-phonon coupling in strongly correlated materials, *Proceedings of the International School of Physics "Enrico Fermi" Course CLXI "Polarons in Bulk Materials and Systems with Reduced Dimensionality"*, Varenna, 21.06-01.07-2005, edited by G. Iadonisi and J. Ranninger, (IOS Press, Amsterdam, 2006) p. 361.
252. G. Sangiovanni, A. Toschi, E. Koch, K. Held, M. Capone, C. Castellani, O. Gunnarsson, S.-K. Mo, J. W. Allen, H.-D. Kim, A. Sekiyama, A. Yamasaki, S. Suga, P. Metcalf: Static vs. dynamical mean field theory of Mott antiferromagnets, *Phys. Rev. B* **73**, 205121 (2006).

253. O. Gunnarsson and O. Rösch: Electron-phonon interaction in the self-consistent Born approximation, *Phys. Rev. B* **73**, 174521 (2006).
254. G. Sangiovanni, O. Gunnarsson, E. Koch, C. Castellani, and M. Capone: Electron-phonon interaction and antiferromagnetic correlations, *Phys. Rev. Lett.* **97**, 046404 (2006).
255. K. Vafayi, M. Calandra, and O. Gunnarsson: Electronic thermal conductivity at high temperatures: Violation of the Wiedemann-Franz law in narrow-band metals, *Phys. Rev. B* **74**, 235116 (2006).
256. O. Rösch, G. Sangiovanni, and O. Gunnarsson: Sum rules and vertex corrections for electron-phonon interactions, *Phys. Rev. B* **75**, 035119 (2007).
257. O. Gunnarsson, G. Sangiovanni, O. Rösch, E. Koch, C. Castellani, and M. Capone: Polaron formation in cuprates, Invited talk at the international conference “Materials and Mechanisms of Superconductivity High Temperature Superconductors VIII”, Dresden, 09-14.07.2006, *Physica C* **460**, 263 (2007).
258. K. Vafayi and O. Gunnarsson: Comment on “Collapse of Coherent Quasiparticle states in Θ -(BEDT-TTF) $_2$ I $_3$ Observed by Optical Spectroscopy”, *Phys. Rev. Lett.* **98**, 219802 (2007).
259. O. Rösch and O. Gunnarsson: Electron-phonon interaction in undoped cuprates: sum rules, vertex corrections and the self-consistent Born approximation, *Physica* **460-462**, 1123 (2007).
260. K. Vafayi and O. Gunnarsson: Analytical continuation of spectral data from imaginary time axis to real frequency axis using statistical sampling, *Phys. Rev. B* **76**, 035115 (2007).
261. G. Sangiovanni and O. Gunnarsson: Electron-phonon interaction in strongly correlated

- electron systems: Relevance of antiferromagnetic correlations. *Journal of Physics: Conference Series* **108**,012012 (2008).
262. O. Gunnarsson and O. Rösch: Interplay between electron-phonon and Coulomb interactions in cuprates, *J. Phys.: Cond. Matt.* **20**, 043201 (2008).
263. O. Gunnarsson: Competition fix, *Nature Materials, News&Views*, **7**, 176 (2008).
264. D. Reznik, G. Sangiovanni, O. Gunnarsson and T. P. Devereaux: Photoemission kinks and phonons in cuprates, *Nature* **455**, E6 (2008).
265. G. Sangiovanni and O. Gunnarsson: Why standard estimates of electron-phonon coupling in cuprates do not work, *Journal of Electron Spectroscopy and Related Phenomena* **181**, 20 (2010).
266. A. Valli, G. Sangiovanni, O. Gunnarsson, A. Toschi, K. Held Dynamic vertex approximation for nanoscopic systems, *Phys. Rev. Lett.* **104**, 246402 (2010).
267. O. Gunnarsson, M.W. Haverkort, G. Sangiovanni: Analytical continuation of imaginary axis data using maximum entropy, *Phys. Rev. B* **81**, 155107 (2010).
268. O. Gunnarsson, M.W. Haverkort, G. Sangiovanni: Analytical continuation of imaginary axis data for optical conductivity, *Phys. Rev. B* **82**, 165125 (2010).
269. O. Gunnarsson, G. Sangiovanni, A. Valli and M. W. Haverkort: Fourier transformation and response functions, *Phys. Rev. B* (submitted).