Dimitrios A. Papaconstantopoulos was born in Athens, Greece, and graduated from the University of Athens with a B.S. degree in Physics in 1961. He received a Ph.D. in theoretical solid state physics from the University of London, England, in 1967. He was a professor of physics at George Mason University from 1967 to 1977 and Chair of the Physics Department from 1974 to 1977. He then joined the Naval Research Laboratory as a government employee. He was director of the Center for Computational Materials Science in the Materials and Technology Division of NRL from 1992 to 2004.
His areas of expertise are in computational condensed matter physics and include band structure calculations, theory of superconductivity, and theory of alloys. He has authored 286 journal articles and three books and has given more than 300 presentations at professional meetings. He has won four Alan Berman Research Publication awards and the 1990 Sigma Xi Pure Science Award at NRL. He has been a Fellow of the American Physical Society since 1980. He has over 10,500 citations in the scientific literature. In August 2000 he was awarded the Navy Meritorious Civilian Service Award. In August 2004 he was appointed as professor of materials science at George Mason where he had held an adjunct professorship since 1992. He has been Chair of the Department of Computational and Data Sciences at George Mason University from January 2006 to December 2010. He has been member of the Computational Materials Science Center (CMaSC) at GMU since 2006.
Currently Professor Emeritus.

EDUCATION

Ph.D. 1967 University of London(U.K.) Theoretical Solid State Physics
M.Sc. 1964 University of London(U.K.) Theoretical Solid State Physics
D.I.C 1963 Imperial College of London Mathematical Physics
B.Sc. 1961 University of Athens (Greece) Physics

POSITIONS HELD

George Mason University:
Chair, Department of Computational and Data Sciences 2006-2010
Professor of Computational Materials Science 2004-2016
Senior Contract Professor, CSI and SCS 1992-2004
Adjunct Professor 1977-1992

Professor and Chair of Physics Department 1974-1977
Associate Professor of Physics 1971-1974
Assistant Professor of Physics 1967-1971
Naval Research Laboratory (NERL):
Research Physicist 1977-2004
Branch Head 1992-2004

PROFESSIONAL SOCIETY MEMBERSHIPS

American Physical Society

HONORS AND AWARDS

- Received publication award for work on the electron-phonon interaction and superconductivity NRL 1975
- Received publication award for work on the electronic structure of A15 compounds NRL 1979
- Elected to Fellowship of the American Physical Society 1980
- Received the Alan Berman publication award for the "Handbook of the Band Structure of Elemental Solids" NRL 1987
- Received the SIGMA XI Pure Science Award NRL 1990
- Received award for NRL Review Article "Solid-State Supercomputing" 1990
- Received award for NRL Review Article "Computational Materials Science" 1994
- Received the Alan Berman publication award for Physical Review article, "Applications of a New Tight-Binding Total Energy Method for Transition and Noble Metals", 1996
- Received the Navy Meritorious Civilian Service Award 2000.
- Certificate of Recognition for "Outstanding Referee" by the American Physical Society, 2008.

PROFESSIONAL DUTIES

- Member of Editorial Board, Journal of Superconductivity, Plenum Publishing edited by D.U. Gubser and S.A. Wolf 1987-95.
- Reviewed extensively for The Physical Review and many other journals.
- Reviewed for several U.S. and European funding agencies.
- Served as the co-organizer and co-chair of the 5th International Conference on "The Physics of Electro-Optic Microstructures and Microdevices 1990.
- Served as the co-organizer and co-chair of the 1st and 2nd International Conferences on "Electronic Structure and Magnetism in Complex Materials" Aug 2000 and July 2002.
- Chair of the Nominating Committee for the APS Div.Comp.Phys. 2000-02
- Member of the Advisory Board of the Materials Science Research Center of

the California State University at Northridge (2002-3)
- Member of the Advisory Board, Philosophical Magazine 2007-2012.

SUPERVISION OF GRADUATE STUDENTS AND POSTDOCS

- Graduated 9 Ph.D. and 3 M.S. students at GMU.
- Served as the co-advisor of four graduate students during sabbatical leaves from NRL in Greece and France.
- Supervised the research of 10 post-doctoral fellows at NRL.

SUMMARY OF RESEARCH OUTPUT

- 286 Articles in refereed journals
- 3 Books
- 155 Invited papers in scientific conferences and university seminars
  210 Contributed talks in meetings

CITATIONS FROM "WEB OF KNOWLEDGE"

- 10,500 citations
- 2,000 citations for the "Handbook of the Band Structure of Elemental Solids"
- H-Index: 42

A. Publications in Refereed Journals

1. "On the Momentum Eigenfunctions for the Periodic Problem," L. Pincherle and D.A. Papaconstantopoulos, Proc. Phys. Soc. Vol. 83, 327 (1964) (London).
2. "Band Calculations for Vanadium," J.R. Anderson, J.W. McCaffrey, and D.A. Papaconstantopoulos, Solid State Commun. 7, 1439 (1969).
3. "Band Structure and Pressure Induced Electronic Transitions in Calcium," J.W. McCaffrey, D.A.Papaconstantopoulos, and J.R. Anderson, Solid State Commun. 8, 2109 (1970).
4. "Band Structure and Fermi Surfaces of Ordered Intermetallic Compounds, TiFe, TiCo, and TiNi," D.A. Papaconstantopoulos and D.J. Nagel, Int. J. Quantum Chem. 5S, 515 (1971).
5. "Self-Consistent Energy Bands in Vanadium at Normal and Reduced Lattice Spacings," D.A. Papaconstantopoulos, J.R. Anderson and J.W. McCaffrey, Phys. Rev. B5, 1214 (1972).
6. "Electronic Structure of Calcium as a Function of the Lattice Constant," J.W. McCaffrey, J.R. Anderson, and D.A. Papaconstantopoulos, Phys. Rev. B6, 674 (1973).
7. "Component Local Densities of States for Ordered TiNi,"

D.A. Papaconstantopoulos, J.W. McCaffrey, and D.J. Nagel, J. Phys. F:Metal Phys. 3, L26 (1973).
8. "Self-Consistent Band Structure of Niobium at Normal and Reduced Lattice Spacings," J.R. Anderson, D.A. Papaconstantopoulos, J.W. McCaffrey, and J.E. Schirber, Phys. Rev. B7, 5115 (1973).
9. "Densities of States and Calculated K X-Ray Spectra of TiFe," D.A. Papaconstantopoulos, Phys. Rev. Lett. 31, 1050 (1973).
10. "Calculated K X-Ray Absorption Spectrum of Calcium," J.W. McCaffrey and D.A. Papaconstantopoulos, Solid state Commun.14,1055,(1974).
11. "Calculations of Crystal Potentials," D.A. Papaconstantopoulos and W.R. Slaughter, Computer Physics Commun. 7, 207 (1974).
12. "Electron-Phonon Interaction and Superconductivity in Transition Metals and Transition Metal Carbides," B.M. Klein and D.A. Papaconstantopoulos, Phys. Rev. Lett. 32, 1193 (1974).
13. "Electronic Structure of TiFe," D.A. Papaconstantopoulos, Phys. Rev. B11, 4801 (1975).
14. "Superconductivity in the Palladium-Hydrogen System," D.A. Papaconstantopoulos and B.M. Klein, Phys. Rev. Lett. 35, 110 (1975).
15. "On Calculating the Electron-Phonon Mass Enhancement for Compounds," B.M. Klein and D.A. Papaconstantopoulos, J. Phys. F:Metal Phys. 6, 1135 (1976).
16. "On the Relationship Between the Phonon Anomalies and the ab initio Calculated Fermi Surfaces of TaC and NbC," B.M. Klein, L.L. Boyer, and D.A. Papaconstantopoulos, Solid State Comm. 20, 937 (1976).
17. "Calculations of the Electron-Phonon Interaction in the Transition Metals, V, Nb, and Ta," L.L. Boyer, B.M. Klein, and D.A. Papaconstantopoulos, Ferroelectrics 16, 291 (1977).
18. "Electronic Structure, Electron-Phonon Interaction and High Temperature Superconductivity in V3Si," B.M. Klein, D.A. Papaconstantopoulos, and L.L. Boyer, Ferroelectrics 16, 299 (1977).
19. "Electron-Phonon Interaction and Superconductivity in Metallic Hydrogen,"D.A. Papaconstantopoulos and B.M. Klein, Ferroelectrics 16,307 (1977).
20. "Effect of Self-Consistency and Exchange on the Electronic Structure of the Transition Metals, V, Nb, and Ta," L.L. Boyer, D.A. Papaconstantopoulos, and B.M. Klein, Phys. Rev. B15, 3685 (1977).

21. "Calculations of the Superconducting Properties of 32 Metals with Z # 49," D.A. Papaconstantopoulos, L.L. Boyer, B.M. Klein, A.R. Williams, V.L. Moruzzi, and
J.F. Janak, Phys. Rev. B15, 4221 (1977).
22. "On the Inverse Isotope Effect and the x-Dependence of the Superconducting Transition Temperature in PdHx and PdDx," B.M. Klein, E.N. Economou, and D.A. Papaconstantopoulos, Phys.Rev.Lett.39, 574, (1977).
23. "Band Structure and Superconductivity of PdDx and PdHx," D.A. Papaconstantopoulos, B.M. Klein, E.N. Economou, and L.L. Boyer, Phys. Rev. B17, 141 (1978).
24. "Self-Consistent APW Band Structure of V3Ga," B.M. Klein, L.L. Boyer, and D.A. Papaconstantopoulos, J. Phys. F 8, 617 (1978).
25. "Isomer Shift and Charge Density in FeAl and the 57Fe Isomer Shift," E.V. Mielczarek and D.A. Papaconstantopoulos, Phys. Rev. B17, 4223 (1978).
26. "Coherent-Potential-Approximation Calculations for PdHx," D.A. Papaconstantopoulos, B.M. Klein, J.S. Faulkner, and L.L. Boyer, Phys. Rev. B18, 2784 (1978).
27. "Calculations of X-Ray Band Spectra; Application to Vanadium," D.A. Papaconstantopoulos, D.J. Nagel, and C.Jones -Bjorklund, Intern. J. Quantum Chem. S 12, 497 (1978).
28. "Band Structure and Electron-Phonon Interaction in Lead," D.A. Papaconstantopoulos, A.D. Zdetsis, and E.N. Economou, Solid State Commun. 27, 1189 (1978).
29. "Self-Consistent APW Electronic Structure Calculations for the A15 Compounds V3X and Nb3X, X=A1, Ga, Si, Ge, and Sn," B.M. Klein, L.L. Boyer, D.A. Papaconstantopoulos, and L.F. Mattheiss, Phys. Rev. B18, 6411 (1978).
30. "Theoretical Calculations of Tc for Lead," A.D. Zdetsis, E.N. Economou, and D.A. Papaconstantopoulos, J. de Physique 40, L-253 (1979).
31. "Superconducting Properties of A15 Compounds Derived from Band-Structure Results," B.M. Klein, L.L. Boyer, and D.A. Papaconstantopoulos, Phys. Rev. Lett. 42, 530 (1979).
32. "Electronic Structure and Superconductivity in Pd-Ag-H and Pd-Rh-H Alloys," D.A. Papaconstantopoulos, E.N. Economou, B.M. Klein, L.L. Boyer, Phys. Rev. B20, 177 (1979).
33. "Spin-Polarized Band Structure Calculations for Ni," J.R. Anderson, D.A. Papaconstantopoulos, L.L. Boyer, and J.E. Schirber,

Phys. Rev. B20, 3172 (1979).
34. "Superconducting Transition Temperatures in Pseudobinary A15 Compounds," D.A. Papaconstantopoulos, D.U. Gubser, B.M. Klein, and L.L. Boyer, Phys. Rev. B21, 1326 (1980).
35. "Ab-Initio Band Structure of Lead," A.D. Zdetsis, D.A. Papaconstantopoulos, and E.N. Economou, J. Phys. F10, 1149 (1980).
36. "Semi-empirical APW Calculation of the Band Structure of Silicon," D.A. Papaconstantopoulos and B.M. Klein, Solid State Commun. 34, 511 (1980).
37. "Slater-Koster Parametrization for Si and the Ideal Vacancy Calculation," D.A. Papaconstantopoulos and E.N. Economou, Phys. Rev. B22, 2903 (1980).
38. "Linear-combination-of-atomic-orbitals-coherent-potential approximations Studies of Carbon Vacancies in the Substoichiometric Refractory Monocarbides NbCx, TaCx, and HfCx," B.M. Klein, D.A. Papaconstantopoulos, and L.L. Boyer, Phys. Rev. B22, 1946 (1980).
39. "Platinum Hydride: A Possible High Temperature Superconductor," D.A.Papaconstantopoulos, J. Less. Comm. Metals 73, 305 (1980).
40. "Theory of Hydrogenated Silicon," E.N. Economou and D.A. Papaconstantopoulos, Phys. Rev. B23, 2042 (1981).
41. "The Superconducting Transition Temperature of Disordered A-15 Compounds," C.M. Soukoulis and D.A. Papaconstantopoulos, Physica B + C, 265 (1981).
42. "Theoretical Prediction of MoN as A High Tc Superconductor," W.E.Pickett, B.M.Klein, and D.A.Papaconstantopoulos, Physica B+C 667,(1981).
43. "Calculations of the Pressure Dependence of the Superconducting Transition Temperature of Vanadium," D.A. Papaconstantopoulos and B.M. Klein, Physica B+C, 107, 725 (1981).
44. "Non-Rigid-Muffin-Tin Calculations of the Electron-Phonon Interaction in Simple Metals," A.D. Zdetsis, E.N. Economou, and D.A. Papaconstantopoulos, Phys. Rev. B24, 3115 (1981).
45. "Calculations of the Electronic Properties of Hydrogenated Silicon," D.A. Papaconstantopoulos and E.N. Economou, Phys.Rev.B24, 7233 (1981).
46. "Influence of Pressure on the Fermi Surface of Niobium," J.A. Anderson, D.A.Papaconstantopoulos, and J.E. Schirber, Phys.Rev.B24,6790 (1981).

47. "Electronic Structure of the Intermetallic Compound TiNi," D.A. Papaconstantopoulos, G.N. Kamm, and P.N. Poulopoulos, Solid State Commun., 41, 93 (1982).
48. "Effects of Disorder on Properties of A15 Materials," C.M. Soukoulis and D.A. Papaconstantopoulos, Phys. Rev. B26, 3673 (1982).
49. "Band Structure and Superconductivity in Bi3Sr and Bi3Eu," D.A. Papaconstantopoulos, B.M. Klein, L.L. Boyer, and J.W.D. Connolly, Phys. Rev. B26, 4951 (1982).
50. "Electronic Structure of Substoichiometric Titanium-Iron Hydride," D.A. Papaconstantopoulos and A.C. Switendick, J. Less. Common. Metals, 88, 273 (1982).
51. "Theoretical Study of Optical Absorption in Hydrogenated Amorphous Silicon," W.E. Pickett, D.A. Papaconstantopoulos, and E.N. Economou, Phys. Rev.B28, 2232 (1983).
52. "Self-Consistent APW Band Structure Calculations of Si and Ge with Overlapping Spheres," D.A Papaconstantopoulos, Phys. Rev. B27, 2569 (1983).
53. "Electronic Structure, Superconductivity and Magnetism in the C15 Compounds ZrV2, ZrFe2, and ZrCo2," B.M. Klein, W.E. Pickett, D.A. Papaconstantopoulos, and L.L. Boyer, Phys. Rev. 27, 6721 (1983).
54. "Slater-Koster Parametrization of the Band Structure of TiNi," J.D. Shore and D.A.Papacostantopoulos, J. Phys. and Chem. of Solids, 45, 439 (1984).
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56. "The Fermi Surface of Iron Under Pressure," W.B. Johnson, J.R. Anderson, and D.A. Papaconstantopoulos, Phys. Rev. B29, 5337 (1984).
57. "Self-Consistent Band Structure Calculations of Titanium, Zirconium, and Hafnium Dihydrides," D.A. Papaconstantopoulos and A.C. Switendick, J. Less. Common. Metals 103, 317 (1984).
58. "Electronic and transport properties of hydrogenated amorphous silicon," A.D. Zdetsis, E.N. Economou, D.A. Papaconstantopoulos, and N. Flytzanis, Phys. Rev. B31, 2410 (1985).
59. "Electronic Properties of Transition Metal Nitrides. The Group V and VI Nitrides VN, NbN, TaN, CrN, MoN, WN," D.A. Papaconstantopoulos, W.E. Pickett, B.M. Klein, and L.L. Boyer, Phys. Rev. B31, 752 (1985).

60. "Calculations of the Electronic Properties of Substoichiometric Ti-Fe Hydride," D.A. Papaconstantopoulos and A.C. Switendick, Phys. Rev. B32, 1289 (1985).
61. "Effects of Disorder on High Temperature Superconductivity in Cubic MoN," D.A. Papaconstantopoulos and W.E. Pickett, Phys. Rev. B31, 7093 (1985).
62. "Superconductivity in Pd-Ag-H Alloys," P.M. Laufer and D.A. Papaconstantopoulos, Physica 135B, 405 (1985).
63. "Systematic Tight-Binding Study of the Electron-Phonon Interaction in Metals," J.L. Fry, G. Fletcher, P.C. Pattnaik, and D.A. Papaconstantopoulos, Physica 135B, 473 (1985).
64. "A Study of various approximations made in APW calculations," N.C. Bacalis, K. Blathras, P. Thomaides, and D.A. Papaconstantopoulos, Phys. Rev. B32, 4849 (1985).
65. "Calculation of Physical Quantities in a-SiHx," E.N. Economou, A.D. Zdetsis, and D.A. Papaconstantopoulos, J. Non-Cryst. Solids 77-78, 147 (1985).
66. "Theoretical Compton Profiles Due to Valence Electrons of Ti and TiH," N.C. Bacalis, N.I. Papanicolaou, and D.A. Papaconstantopoulos, J. Phys. F16, 1471 (1986).
67. "Theory of Superconductivity in Palladium-Noble-Metal Hydrides," P.M. Laufer and D.A. Papaconstantopoulos, Phys. Rev. B33, 5135 (1986).
68. "Calculation of Compton Profiles of Tantalum and Tungsten," N.I. Papanicolaou, N.C. Bacalis, and D.A. Papaconstantopoulos, Phys. Status Solidi (b) 137, 597 (1986).
69. "Electronic Structure of the Fe/Ge (110) Interface," W.E. Pickett and D.A. Papaconstantopoulos, Phys. Rev. B34, 8372 (1986).
70. "Transferability and Scaling of Slater-Koster Parameters in Transition Metals," J.D. Shore and D.A. Papaconstantopoulos, Phys. Rev. B35, 1122 (1987).
71. "Calculation of the Compton Profiles of Vanadium, Niobium, and their Dihydrides," N.I. Papanicolaou, N.C. Bacalis, and D.A. Papaconstantopoulos, Z. Phys. B65, 453 (1987).
72. "Calculations of the Electronic Structure and Disordered Transition Metal Dihydrides," D.A. Papaconstantopoulos and P.M. Laufer, J. Less. Common. Metals, 130, 229 (1987).
73. "Electronic Structure and Magnetic Effects at the Ideal (110) Fe/Ge Interface," W.E. Pickett and D.A. Papaconstantopoulos, J. Appl. Phys. 61, 3735 (1987).

74. "Tight-Binding Coherent-Potential-Approximation Study of the Electronic States of Palladium-Noble Metal Alloys," P.M. Laufer and D.A. Papaconstantopoulos, Phys. Rev. B35, 9019 (1987).
75. "Evidence of Conventional Superconductivity in La-Ba-Cu-O Compounds," W.E. Pickett, H. Krakauer, D.A. Papaconstantopoulos, and L.L. Boyer, Phys. Rev. B35, 7252 (1987).
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77. "Band Structure and Electron-phonon Interaction of LaAgO3," N.C. Bacalis and D.A. Papaconstantopoulos, J.of Superconductivity, 1,175, (1988).
78. "Tight-binding Study of the Electron-Phonon Interaction in BCC Transition Metals and Alloys," G. Fletcher, J.L. Fry, P.C. Pattnaik, D.A.Papaconstantopoulos, and N.C. Bacalis, Phys. Rev. B37, 4944 (1988).
79. "Magnetism in BCC and FCC Manganese," G. Fuster, N.E. Brener, J. Callaway, J.L. Fry, Y.Z. Zhao, and D.A. Papaconstantopoulos, Phys. Rev. B38, 423 (1988).
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83. "Calculations of the Electronic Structure of La2-xMxCuO4-y by the Coherent Potential Approximation," D.A. Papaconstantopoulos, W.E. Pickett, and M.J. DeWeert, Phys. Rev. Lett. 61, 211 (1988).
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86. "First-Principles Study of LlO Ti-Al and V-Al Alloys," S.R. Chubb, D.A. Papaconstantopoulos, and B.M. Klein, Phys.Rev.B38, 12120,

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88. "Ferromagnetism in Hexagonal-Close-Packed Elements," D.A. Papaconstantopoulos, J.L. Fry, and N.E. Brener, Phys.Rev.39, 2526, (1989).
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91. "Tight-binding-coherent-potential approximation calculations in Cu-Pd including off-diagonal disorder," D.A. Papaconstantopoulos, A. Gonis, and P.M. Laufer, Phys. Rev. B40, 12196 (1989).
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99. "Magnetism in Layered Oxides: Results from Spin Density Functional Calculations," D. Singh, W.E. Pickett, R.E. Cohen, D.A. Papaconstantopoulos and H. Krakauer, Physica B 163, 478 (1990).
100."Possibility of LiPdHx as a new ionic superconductor?" D. Singh, R.E.Cohen and D.A.Papaconstantopoulos, Phys.Rev.B41, 861, (1990).
101."Structural Properties of Ordered High-Melting-Temperature Metallic Alloys from First Principles Total Energy Calculations," M.J. Mehl, J.E. Osburn, D.A. Papaconstantopoulos, and B.M. Klein, Phys. Rev. B41, 10311 (1990); erratum Phys. Rev. B42, 5362 (1990).
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115."Comment on Total Energy Calculations of Solid H, Li, Na, K, Rb and Cs," D.A. Papaconstantopoulos and D.J.Singh, Phys.Rev.B45,7507,(1992).
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244. "The SlaterKoster Tight-Binding Method: A Computationally Efficient and Accurate Approach," D.A. Papaconstantopoulos and M.J. Mehl, J.Phys: Condens. Matter 15, R413R440 (2003). Review
245. "Tight-Binding Total Energy Methods for Magnetic Materials and Multi-element Systems," M. J. Mehl and D. A. Papaconstantopoulos, in Handbook of Materials Modeling, Volume I: Methods and Models, S. Yip, editor Volume I: Methods and Models, S. Yip, edit. pp 275-305 (2005).
246. "Tight-Binding Method in Electronic Structure," D.A. Papaconstantopoulos, and M.J. Mehl, in "Encyclopedia of Condensed Matter Physics," Vol 6, pp 194-206, Elsevier, (2005).
247. "An Introduction to Electronic Structure Methods," D. A. Papaconstantopoulos, in Complex Metallic Alloys Series-Vol 1, Basics of thermodynamics and phase transitions in complex materials, Chapter 8, pp 189-218, World Scientific, (2008).
248. "Handbook of the Band Structure of Elemental Solids: From Z=1 To Z=112", D.A. Papaconstantopoulos, Springer 2015.

C. Conference Proceedings Papers

249. "Calculated X-Ray Band Spectra," D.J. Nagel, D.A. Papaconstantopoulos, J.W. McCaffrey, and J.W. Criss, "Proceedings of Int. Symposium on X-Ray Spectra and Electronic structure of Matter," ed. by A. Faessler and G. Wiech, Vol. 2, 51 (1973).

250. "Calculations of the Electron-Phonon Interactions and Superconductivity in the Palladium-Hydrogen System," B.M. Klein and D.A. Papaconstantopoulos, Proceedings of the 14th Int. Conf. on Low Temperature Physics, Helsinki, Finland, ed. by M. Krusius and M. Vuorio, Vol. 2, 399 (1975).
251. "Calculations of X-Ray Band Spectra," Intern. Conf. on the Physics of X-Ray Spectra, D.A. Papaconstantopoulos, National Bureau of Standards Pub., p. 192 (1976).
252. "Calculations of the Superconducting Properties of Compounds: Refractory Carbides, PdH and V3Si," B.M. Klein, D.A. Papaconstantopoulos, and L.L. Boyer, Proceedings of the 2nd Rochester Conf. on Superconductivity in d-and f- Band Metals, ed. by D.H. Douglass, Plenum Press, p. 339-359 (1976).
253. "Bonding in Transition Metal Aluminides," D.J. Nagel, L.L. Boyer, D.A. Papaconstantopoulos, and B.M. Klein, Inst. Phys. Conf. Ser. No. 39, p. 104 (1978).
254. "Superconductivity in Palladium-Based Hydrides," D.A Papaconstantopoulos, E.N. Economou, B.M. Klein, and L.L. Boyer, J. de Physique C-6, 435 (1978).
255. "Electronic Structure, Electron-Phonon Interactions and Low Temperature Anomalies in A15 Compounds," B.M. Klein, L.L. Boyer, and D.A. Papaconstantopoulos, J. de Physique C-6, 416 (1978).
256. "Coherent-Potential Approximation Studies of Carbon Vacancies in the Transition-Metal Monocarbides," B.M. Klein, D.A. Papaconstantopoulos, and L.L. Boyer, Proceedings of AIME Annual Meeting, Theory of Alloy Phase Formation, ed. by L.H. Bennett,p.479 (1979).
257. "Calculations of the Superconducting and Transport Properties of A15 Structure Compounds," B.M. Klein, D.A. Papaconstantopoulos, L.L. Boyer, Proceedings of the 3rd Conference on Superconductivity in d and f-band Metals, ed. by H. Suhl and M.B. Maple, Academic Press pp. 455-464 (1980).
258. "Calculations of the Superconducting Properties of NbC1-xNx," D.A. Papaconstantopoulos, Inst. Phys. Conf. Ser. No. 55, 563 (1981).
259. "Coherent-Potential-Approximation Calculations of the Electronic Properties of the Substoichiometric Refractory Monocarbide NbCx, TaCx, and HfCx," B.M. Klein, D.A. Papaconstantopoulos, and L.L. Boyer, Inst. Phys. Conf. Ser. No. 55, 53 (1981).
260. "Electronic Densities of States in a-Si:H," D.A. Papaconstantopoulos and E.N. Economou, AIP Conf. Proceedings

No. 73, 130 (1981).
261. "Calculations of Transport Properties in a-Si:H," W.E. Pickett, D.A. Papaconstantopoulos, and E.N. Economou, Proc. 9th Intern. Conf. on Amorphous and Liquid Semiconductors (1981) and J.de Physique,42, C4-769,(1981).
262. "Electron-Phonon Interaction in Transition Metal Dihydrides," D.A. Papaconstantopoulos, LT-17 Proceedings, eds. U. Eckern, A. Schmid, W. Weber, H. Wiehl, p. 129, North-Holland (1984).
263. "Calculations of the Electronic and Transport Properties in Si-Ge-H Alloys," D.A. Papaconstantopoulos, E.N. Economou, and A.D. Zdetsis, Proc. 17th Intern. Conf. on Physics of Semiconductors, ed. J.D. Chadi and W.A. Harrison, 795, Springer- Verlag, NY (1985).
264. "Electronic Structure and Interface States of the (110 Fe/Ge Interface," W.E. Pickett and D.A. Papaconstantopoulos, 18th Intern. Conf. on the Physics of Semiconductors, p. 351, World Scientific (1987).
265. "Electronic Structure, Bonding and Electron-Phonon Interaction in La-Ba-Cu-O Superconductors," W.E. Pickett, H. Krakauer, D.A. Papaconstantopoulos, L.L. Boyer and R.E. Cohen, in High Temperature Superconductors, edited by D.U. Gubser and M. Schluter (Mat. Res. Soc., Pittsburgh, 1987), p.31.
266. "Band Structure and Electron-Phonon Interaction Calculations for Proposed High- Tc Superconducting Oxides: MCUO3 (M = LA, BA, CS, Y) in the Perovskite Structure," D.A. Papaconstantopoulos and L.L. Boyer, Novel Superconductivity, edited by S.A. Wolf and V.Z. Kresin (Plenum, 1987), p. 493.
267. "High Temperature Superconductors: Electronic Structure Changes due to Replacement of La with Ba and Sr in the Cu-O-Based Systems," H. Krakauer, W. E. Pickett, D. A. Papaconstantopoulos and L. L. Boyer, Proc. 18th Int. Conf. on Low Temperature Physics, Kyoto, 1987, Jap. J. Appl. Phys., Supplement 26-3, 991-2 (1987).
268. "Calculations of the Superconducting Properties of Cu-O Based Perovskite-Like Structures," D. A. Papaconstantopoulos, W. E. Pickett, H. Krakauer and L. L. Boyer, Proc. 18th Int. Conf. on Low Temperature Physics, Kyoto, 1987, Jap. J. Appl. Phys., Supplement 26-3, 1091-2 (1987).
269. "Tight-Binding Study of the Electronic Structure of the High Temperature Superconductor," D.A. Papaconstantopoulos, M.J. DeWeert and W.E. Pickett, Mat. Res. Soc. Symp. Proc. 99, 447

(1988).
270. "Applicability of Conventional Band Theory and the Role of Phonons in High Tc Superconductors," R.E. Cohen, D. Singh, W.E. Pickett, D.A. Papaconstantopoulos, H. Krakauer, and P.B. Allen, Proceedings of High Tc Superconductors: Magnetic Interaction, Progress in Superconductors, Ed.L. H. Bennett, Y. Flom, and G.C. Vezzoli, Vol. 17, P. 93-105 (1989).
271. "A Tight-Binding Hamiltonian for the High-Temperature Superconductor YBa2Cu3O7," M.J. DeWeert, D.A. Papaconstantopoulos and W.E. Pickett, MRS Symp.Proc. Vol. 141, p. 103 (1989).
272. "Accurate Tight-Binding Studies of Antiferromagnetic States of La2CuO4," W.E. Pickett and D.A. Papaconstantopoulos, MRS Symp. Proc., Vol. 141, p 109, (1989).
273. "GaAs Tight-Binding Hamiltonians," J. Broughton, D.A. Papaconstantopoulos, M. Pederson and D. Singh, "The Physics of Semiconductors" Vol. 3, p. 1771, eds. Anastassakis and Joannopoulos, World Scientific (1990).
274. GaAs Total Energy Tight Binding Hamiltonians for Use in Molecular Dynamics," J. Broughton, M. Pederson, D.A. Papaconstantopoulos and D. Singh, MRS Symp. Proc. Vol. 193, 219 (1990).
275. "Electronic Structure of Copper Free Superconductors and Related Compounds," J.P. Julien, D.A. Papaconstantopoulos, F. Cyrot-Lackmann, D. Mayou, Proc. Int'l. Conf. Materials & Mechanisms of Superconductivity High-Temp. Superconductors, Kanazawa, Japan (1991).
276. "First Principles Calculations of the Equilibrium Mechanical Properties of Simple Metals and Ordered Intermetallic Alloys," M.J. Mehl, J.E. Osburn, D.A. Papaconstantopoulos and B.M. Klein, MRS Symp. Proc. Vol. 186, 277 (1991).
277. "Coupling of Octahedral Tilts to the Electronic Structure in La2-x(Sr,Ba)xCuO4," R.E. Cohen, W.E. Pickett, D.A. Papaconstantopoulos and H. Krakauer, Lattice Effects in High-Tc Supercomputers, Eds. Y. Bar-Yam, T. Egami, J. Mustre-de Leon and A.R. Bishop (World Scientific, 1992) p. 223.
278. "Transferable Total Energy Parametrization for Metals," M. Sigalas and D.A.Papaconstantopoulos, Mat.Res.Soc.Symp.Proc.291, 27, (1993).
279. "Towards Calculations of the Total Energy of Large Systems,"

D.A. Papaconstantopoulos, M.J. Mehl, M.M. Sigalas and M.A. Keegan, "Metallic Alloys: Experimental & Theoretical Perspectives, Faulkner & Jordan (eds.), Kluwer Academic Pub., 451 (1994).
280. "First-Principles Tight-Binding Total Energy Calculations for Metals," M.J. Mehl, D.A. Papaconstantopoulos, R.E. Cohen and M.M. Sigalas, Alloy Modelling and Design, G.M. Stocks and P.E.A. Turchi, eds., Minerals, Metals and Materials Soc., 25 (1994).
281. "Equation of State for PdH by a New Tight-Binding Approach," D.A. Papaconstantopoulos and M.J. Mehl, Mat. Res. Soc. Symp. Proc. 408, 31 (1996).
282. "Applications of a New Tight-Binding Total Energy Method," D.A.Papaconstantopoulos, M.J. Mehl and B.Akdim, Proceeedings of the Intern. Symposium on Novel Materials, Bhubaneswar, India, p. 393-403 (1998).
283. "Tight-Binding Hamiltonians for Carbon and Silicon," D.A. Papaconstantopoulos, M.J. Mehl, S.C. Erwin and M.R. Pederson, Mat. Res. Soc. Symp., 491, 221 (1998).
284. "From ab initio calculations to disslocation behavior using interatomic potentials"Y. Mishin, D. Farkas, M.J. Mehl and D.A. Papaconstantopoulos Mat.Res.Soc.Symp.Proc.408 (1999)
285. "Lattice Trapping of Cracks in Fe Using an Interatomic Potential Derived From Experimental Data and Ab Initio Calculations," D. Farkas, M. J. Mehl, and D. A. Papaconstantopoulos, in Multiscale Modeling of Materials--2000, L.P. Kubin, J.L. Bassani, K. Cho, H. Gao,R.L.B. Selinger, eds. Mat. Res. Soc. Symp. Proc. 653, Z6.4 (2001).
286. "Structural and electronic properties of V, Nb and Ta nanoclusters by tight-binding molecular dynamics simulations," Ch.E. Lekka, and D.A. Papaconstantopoulos, Surface Science, Volume 601, Issue 18, Pages 3937-3942 ,(2007). ECOSS-24, Proceedings of the 24th European Conference on Surface Science

INVITED TALKS

1. "Band Structure in 3d Metal Compounds," National Bureau of Tandards, Institute for Materials Research, (November 1971).
2. "Calculations with the APW Method," University of Virginia,

Charlottesville, Department of Physics, (March 1972).
3. "Energy Bands and X-Ray Spectra with the APW Method, "Department of Physics Bedford College of the University of London, (June 1972).
4. "Band Theory of Solids," 10 lectures, Summer Institute Nuclear Research Center, "Demokritos," Athens, Greece, (July and August 1972).
5. "Superconductivity in Transition Metals and Transition Metal Carbides," International Symposium on Atomic Molecular and Solid State Theory, Sanibel Island, Florida, (January 1974).
6. "Electron-Phonon Interaction and Superconducting Transition Temperatures from Augmented Plane Wave Calculations," Naval Research Laboratory, (March 1974).
7. "Electron-Phonon Interaction and Superconducting Transition Temperatures from Energy Band Structure Calculations,"Jet Propulsion Laboratory, Pasadena,(1974).
8. "Calculations of Tc in Transition Metals and Transition Metal Compounds," University of Virginia, Charlottesville, Department of Physics, (Sept 1974).
9. "Band Structure and Superconductivity in Transition Metals and Transition Metal Carbides," University of Maryland, Department of Physics, (October 1974).
10. "Self-Consistent Energy Bands and Superconductivity in PdH," International Symposium on Atomic Molecular and Solid State Theory, Sanibel Island, FL, (Jan 1975).
11. "Calculations of the Electron-Phonon Interaction from Band Structure Results," Virginia Polytechnic Institute and State University, Department of Physics, (October 1975).
12. "Calculations of the Electron-Phonon Interaction and Superconducting Transition Temperature in Metals and Compounds," Naval Research Laboratory, Washington, DC, (December 1975).
13. "Calculations of the Electron-Phonon Interaction and Superconducting Transition Temperature in Metals and Compounds," 13th Annual Solid State Physics Conference, Manchester, England, (January 1976).
14. "Calculations of X-Ray Band Spectra," International Conference on the Physics of X-Ray Spectra, National Bureau of Standards, Gaithersburg, MD., (September 1976).
15. "Superconductivity in the Pd-H and the Pd-Ag-H Systems," International Workshop on Phonons, Paris, France, (August 1977).

16. "Band Structure and Superconductivity in Palladium-Hydride," Univ. of Maryland, Dept. of Physics, (October 1977).
17. "Calculations of the Superconducting Properties of Metals and Compounds," National Science Foundation, Washington, DC, (February 1978).
18. "Calculations of X-Ray Spectra in A-15 Compounds," International Symposium on Atomic, Molecular, and Solid State Theory, Daytona, Florida, (March 1978).
19. "Hydrides," ONR-NRL Superconducting Materials Symposium, Washington, DC, (September 1978).
20. "Electron-Phonon Interaction in Complicated Structures," Oak Ridge National Laboratory, Oak Ridge, TN, (December 1978).
21. "Electron-Phonon Interaction in Metal Hydrides and A-15 Compounds," Univ. of Virginia, Dept. of Physics, (December 1978).
22. "Superconducting Properties of Metal Hydrides and A-15 Compounds," Univ of Karlsruhe, Karlsruhe, Germany, (March 1979).
23. "Electron-Phonon Interaction in Metal Hydrides," 2nd Biennial High Pressure Symposium, Watervliet Arsenal, NY (June 1979).
24. "Band Theory of Hydrogenated Metals and Semiconductors," Dept. of Physics, Univ. of Wyoming, (November 1979).
25. "Theory of Hydrogenated Silicon," Exxon Laboratories, Linden NJ, (May 1980).
26. "Theory of Hydrogenated Silicon," Energy Conversion Devices Inc., Detroit, MI, (June 1980).
27. "Band Structure of Metal Hydrides," NATO Advanced Study Institute, Rhodes, Greece, (June 1980).
28. "Electronic Structure of Si with Vacancies and Hydrogen," Dept. of Physics University of Bristol, England, (August 1980).
29. "Electronic Densities of States in -Si: H," Dept. of Physics, Univ. of Illinois, Urbana, IL, (3 April 1981).
30. "Electronic Densities of States in -Si:H," Dept. of Physics, Univ. of Virginia, Charlottesville, VA, (16 April 1981).
31. "Electronic Structure of Transition-Metal Carbides, Nitrides and Borides," Joint Fall Mtg. Am. Met. Soc. Louisville, KY, (October 1981).
32. "Calculations of the Electronic Properties of Hydrogenated Amorphous Silicon," IBM, Yorktown Hghts., NY, (28 June 1982).
33. "Electronic Structure of Substoichiometric Titanium-Iron Hydride," Intern. Symp. on the Properties and Applications of Metal Hydrides II, Toba, Japan, (Jun 1982).
34. "Electronic Structure of Substoichiometric Carbides and

Hydrides," Alloy Theory and Development Workshop, (8-10 Sept. 1982), Los Alamos National Lab.
35. "Calculations of the Electronic Properties of Hydrogenated Amorphous Silicon," Sandia Lab., Albuquerque, NM, (7 Sept. 1982).
36. "Calculations of the Electronic Structure of Substoichiometric Transition Metal Hydrides," APS, San Francisco, CA, (20-23 Nov. 1983).
37. "Applications of Band Theory in Superconductivity," National Research Council, Athens, Greece, (5 Jan. 1984).
38. "Application of Band Theory in Amorphous Semiconductors," University of Crete, Heraklion, Crete, Greece, (18 Feb. 1984).
39. "Superconducting Properties of Metal Hydrides," XVII International Conference on Low Temperature Physics, Karlsruhe, Germany, (20 Aug 1984).
40. "Exploring Possibilities for High Temperature Superconductivity in Transition Metal Nitrides," Oak Ridge National Lab, Oak Ridge (Nov. 1984).
41. "Will Disorder Destroy High Temperature Superconductivity in Cubic MoN?," Univ. of Texas, Arlington, TX, (27 Nov. 1984).
42. "Superconducting Properties of Metal Hydrides," D.A. Papaconstantopoulos, Virginia Commonwealth Univ., Richmond, VA, (May 1985).
43. "Theory of Electronic States in Disordered Alloy Hydrides," NATO ASI on Hydrogen in Disordered and Amorphous Solids, Rhodes, (Sept 1985).
44. "Effective-Medium Theory of Alloy Electronic Structure: LCAO-CPA," Intern. Workshop on the Electronic Structure of Defects in Metals and Alloys, Argonne, (June 1986).
45. "Recent Advances in the Theory of the Electronic Structure of Solids," 2nd Annual Meeting of the Physics of Condensed Matter, Univ. of Ioannina, Greece, (Sep 1986).
46. "Theory of High Temperature Superconductors," Workshop on "Electronic Structure and Atomic Dynamic Simulated Annealing," Brookhaven Lab., (March 1987).
47. "Theory of the Electronic and Superconducting Properties of La (M)-Cu-O," APS Meeting, New York, (March 1987).
48. "Electronic Properties of Transition Metal Carbides and Nitrides," MRS Meeting, Anaheim, CA, (April 1987).
49. "New High Temperature Superconductors," Dept. of Physics, George Mason University, Fairfax, VA, (May 1987).

50. "High Temperature Superconductivity," Dept. of Physics, University of Crete, (June 1987).
51. "High Temperature Superconductivity," National Hellenic Research Foundation, Athens, (June 1987).
52. "High Temperature Superconductivity," University of Patras, Greece, (June 1987).
53. "Electronic Structure Studies in Metallic Alloys and High Temperature Superconductors," Laboratoire de Chimie Physique, Universite Pierre et Marie Curie, Paris, France, (Sept. 1987).
54. "Electronic Structure of Hydrogenated Amorphous Silicon," Ecole Polytechnique, Paris, France, (Sept. 1987).
55. "Electronic Structure Studies in Disordered Materials and High Temperature Superconductors," Louisiana State Univ., Baton Rouge, LA, (February 1988).
56. "Recent advances in high temperature superconductivity," Nuclear Research Center Dimokritos, Athens, Greece, (February 1988).
57. "Theories of High Temperature Superconductors," 4th Panhellenic Conference on Solid State Physics, Marathon, Greece, (September 1988).
58. "Electronic Structure of the High Temperature Superconductors," Laboratory for Studies of the Electronic Properties of Solids, Grenoble, France, (Oct 1988).
59. "Predictions of Ferromagnetism in HCP Metals," Laboratory for Studies of the Electronic Properties of Solids, Grenoble, France, (Mar 1989).
60. "Electronic Structure of Intermetallic Alloys," Workshop on Computational Methods for the Electronic Structure of Metallic Alloys, University of Kentucky, Lexington, (May 1989).
61. "What Band Theory Can Tell Us About Metal Hydrides," Gordon Research Conference on Metal Hydrides, Tilton, NH, (July 1989).
62. "Computational Theory of High Temperature Superconductors," Dept. of Physics, Virginia Commonwealth University, Richmond, VA, (October 1989).
63. "Band Structure Engineering," George Mason Univ. Fairfax, VA, (Mar 1990).
64. "Systematic Studies of the Electronic Properties of Transition-Metal Compounds," Workshop on Computational Methods for the Electronic Structure of Metallic Alloys, Univ. of Kentucky, Lexington, (June 1990).

65. "Calculations of the Total Energy, Electron-Phonon Interaction and Stoner Parameter in Transition Metal Hydrides," Int'l. Symp. on Metal Hydrogen Systems; Fundamentals and & Applications, Banff, Alberta, Canada, (1-7 Sep 1990).
66. "Total Energy Calculations and Other Good Things" Workshop on Computational Methods in the Theory of Alloys, Univ. of Kentucky, Lexington, KY, (June1991).
67. "Magnetism in Transition Metal Hydrides" University of Crete, Greece, (July 1991).
68. "Total Energy and Electronic Studies in Aluminides, Hydrides, Carbides, Nitrides and Oxides," Sandia National Laboratory, Albuquerque, NM, (January 1992).
69. "First Principles Quantum Mechanics for Real Systems," George Mason University, (January 1992).
70. "Calculations of Electronic and Mechanical Properties of Solids from First Principles," Universite Pierre et Marie Curie, Paris, France, (February 1992).
71. "Total Energy and Electronic Structure Studies of Metal-Hydrogen Systems," March APS Meeting, Indianapolis, IN, (March 1992).
72. "First Principles Calculation of Elastic Constants" NATO Advanced Institute on Statics and Dynamics of Alloy Phase Transformations, Rhodes, (June 1992).
73. "Electronic Structure of Solids," University of Crete, Heraklion, (July 1992).
74. "Electronic Structure of Solids," National Hellenic Research Foundation, Athens, (July 1992).
75. "Electronic Structure of Nitrides," Gordon Conference Solid State Chemistry, Plymouth, NH, (July 1992).
76. "Towards Calculations of the Total Energy of Very Large Systems, 6th Annual Workshop on Comp. Methods for the Structure of Alloys, Lexington, KY, (June 1993).
77. "Calculations of Elastic Constants and Phonon Spectra," NATO Advanced Study Institute on Nanophase Materials, Corfu, Greece, (June 1993).
78. "Towards Calculations of the Total Energy of Large Systems," NATO Advanced Research Workshop, Metallic Alloys: Experimental and Theoretical Perspectives, Boca Raton, FL, (July 1993).
79. "A New Tight-Binding Total Energy Method for Transition and Noble Metals," Ames Lab., Iowa State Univ., Ames, IA, (April 1994).
80. "A New Tight-Binding Total Energy Method for Transition and

Noble Metals," Workshop on computational methods for the Structure & Dynamics of Solids, Lexington, KY, (May 1994).
81. "Tight-Binding Total Energy Calculations for Metals," George Mason University, Fairfax, VA, (November 1994).
82. "Tight-Binding Total Energy Calculations for Metals," Virginia Polytechnic Inst. and State Univ., Blacksburg, VA, (November 1994).
83. "Tight-Binding Total Energy Calculations for Metals," 1995 TMS Meeting "Hume-Rothery Award Symposium," Las Vegas, NV, (February 1995).
84. "Tight-Binding Total Energy Calculations for Metals," Workshop on Electronic Structure Theory, Univ. of Calif. Davis, Davis, CA, (Mar 1995).
85. "New Methodology for Total Energy Calculations," NATO ASI on "Stability of Materials," Corfu, Greece, (July 1995).
86. "New Developments in Tight Binding Calculations," Demokritos Research Center, Athens, Greece, (July 1995).
87. "New Development in Tight-Binding Technology for Calculating Total Energies of Solids," European Phys. Soc. 15th Gen. Conf. Of Condensed Matter Div., Lago Maggiore, Italy, (April 1996).
88. "New Developments in Tight-Binding for Calculating Total Energies," Pierre et Marie Curie University, Paris, France, (April 1996).
89. "New Developments in Tight-Binding for Calculating Total Energies," University of Paris (Orsay), (April 1996).
90. "New Developments on Tight-Binding Calculations," LEPES-CNRS, Grenoble, France, (May 1996).
91. "Tight-Binding Interpolation," IRMA, Lausanne, Switzerland, (May 1996).
92. "Tight-Binding Interpolation," Max Planck Institute, Stuttgart, Germany, (May 1996).
93. "A New Tight-Binding Methodology for Calculating Total Energies," Oxford, England, (May 1996).
94. "Tight-Binding Interpolation," CECAM Workshop, Lyon, France, (June 1996).
95. "Tight-Binding Technology for Calculating Total Energies of Solids," First Intnl. Alloy Conference, Athens, Greece, (June 1996).
96. "New Calculation Methodology of the Total Energy of Solids," XII Greek Solid State Physics Conference, Heraklion, Crete, Greece, (September 1996).
97. "The Tight-Binding Method as a Tool for Materials Design," Intnl.

Symp. On Novel Materials, Puri, India, (March 1997).
98. "Tight-Binding Total Energy Calculations," Workshop on Interatomic Potentials and Linking Scales, Univ. Of California, Santa Barbara, CA, (June 1997).
99. "A Tight-Binding Scheme Applicable to Surfaces," Euroconference Corfu 97, Corfu, Greece, (June 1997).
100. "Tight-Binding Molecular Dynamics," CHSSI CCM Workshop, Dayton, OH, (August1997).
101. "A New Computational Methodology for Calculating Total Energies in Solids" Univ. Of Delaware, Newark, DE, September 1997.
102. "Tight-Binding Interpolation of First-Principles Total Energies," MRS Fall Meeting, Boston, MA, (December 1997).
103. "The NRL Tight-Binding Method, UC Davis Workshop on Materials Theory," Univ. of Calif., Davis, (March 1998).
104. "First-Principles Calculations in Materials Science," TTCP MAT Meeting, DERA, Farnborough, England, (April 1998).
105. "Tight-Binding Interpolation of First-Principles Total Energies," Physics Dept., Imperial College, London, UK, (April 1998).
106. "The NRL Tight-Binding Method Applied to Semiconductors," Intl. Conference on Correlation Effects and Materials, Heraklion, Crete, Greece, (June 1998).
107. "The NRL Tight-Binding Method," Intl. Workshop on Massively Parallel and Superscalar Applications in Computational Materials Science, Paderborn, Germany, (August 1998).
108. "Recent advances in computational materials science," George Mason Univ (Nov 1998).
109. "Tight-binding interpolation of first-principles total energies," Saclay Nuclear Research Center, Paris, France, (February 1999).
110. "Materials Science using elaborate tight-binding Hamiltonians," Pierre et Marie Curie University, Paris France, (January 1999).
114. "The NRL Tight-Binding Method," Workshop on Probing Potential Energy Surfaces, Zermatt, Switzerland, (April 1999).
116."Tight-binding method for metals, insulators, and semiconductors" 2nd International Alloy conference, Davos, Switzerland (August 1999).
117."Tight-binding Hamiltonians in Solids," Mardi Gras 2000 Materials Design: Experimental and Computational Challenges, Baton Rouge (March 2000).
118. "Tight-binding Schemes for Semiconductors and Metals," Symposium on Wave Propagation and Electronic Structure in

Disorder Systems, Heraklion Crete (June 2000).
119. "Tight-binding Method: Connections to First Principles and to Molecular Dynamics," 1st Intern. Confer. on Multiscale Materials Phenomena, Limassol, Cyprus, (June 2000).
120."Computational Materials Science from First Principles," National Research Council, Washington DC (March 2001).
121. "Computational Materials Science from First Principles," DOD Computational Materials Science Workshop, St. Louis, (April 2001).
122."The NRLTB Method; The Road to Large Scale Electronic Structure and Total Energy Calculations," Dept. of Physics Harvard University, (May 2001).
123."Computational Materials Science," Laboratory of Physical Chemistry, Pierre et Marie Curie University, Paris, France, (June 2001).
124."A Tight-Binding Approach Exceeding the Limits of First Principles Calculations," CECAM Workshop on Rigidity and Strain Fields in Crystalline and Amorphous Materials, Lyon, France, (June 2001).
125."The NRLTB Method; The Road to Large Scale Electronic Structure and Total Energy Calculations," Grenoble, France, (June 2001).
126."Extensions of the NRLTB Scheme to Magnetic Materials and Binary Systems," CECAM Workshop on Multiscale Modeling of Materials, Crete, Greece, (July 2001).
127."The NRLTB Method; The Road to Large Scale Electronic Structure and Total Energy Calculations," National Hellenic Research Foundation, Athens, Greece, (July 2001).
128."The NRLTB Method; The Road to Large Scale Electronic Structure and Total Energy Calculations," VII International Conference on Advanced Materials ICAM 2001, Cancun, Mexico, (August 2001).
129."Linking APW Calculations to Tight-Binding," Workshop on NanoAl, Corfu, Greece, (September 2002).
130. "Tight-binding v. LDA+U in FeAl and MnAl," Realistic Theories of CEM, Santa Barbara, (November 2002).
131. "The NRLTB Method; Applications to Binary and Ternary Systems," Calphad XXXII, La Malbaie, Quebec, Canada, (May 2003).
132. "Improvements to Harrison's Tight-binding Theory," XII International Materials Research Congress, Cancun, Mexico, (August 2003).

133. "Tight-binding Simulations of the Various Polytypes of SiC," NN2003, International Conference on Nanomaterials and Nanotechnologies, Crete, Greece, (September 2003).
134. "Tight-binding Methodologies for Efficient Electronic Structure and Total Energy Evaluations," 2003 Computational Chemistry Conference on Software Solutions to Large Scale Problems in Computational Chemistry, University of Kentucky, Oct 2021, 2003.
135."Tight-binding Methodologies for Efficient Electronic Structure and Total Energy Calculations," Workshop on Hierarchical Modeling and Multiscale Simulation of Materials Interfaces, University of Maryland, Oct 2731, 2003.
136."Transformation of Harrison's Tight-binding Theory from a Qualitative Approach to a Quantitative Tool," MRS Meeting, Boston, (December 2003).
137."Recent Applications of the NRLTB Method," 44th Sanibel Symposium, St. Augustine, Fl, (February 2004).
138. "Realistic Tight-binding Methodologies," Fourth International Alloy Conference (IAC4), Kos, Greece, (June 2005).
139."Large-Scale Calculations with a Tight-Binding Approach," XIV, International Materials Research Congress, Cancun, Mexico, (August 2005).
140."An Introduction to Electronic Structure Methods," 1st Euroschool in Materials Science, (22 May 2006), Ljubljana, Slovenia.
141."Tight-binding Methodologies in Electronic Structure," 1st Euroschool in Materials Science, (23 May 2006), Ljubljana, Slovenia.
142."Theoretical Predictions of Superconductivity in Alkali and Other Simple Metals," The 8th International Conference on Materials and Mechanisms of Superconductivity (M2S-HTSC VIII), (9-14 July 2006), Dresden, Germany.
143."Effects of Pressure on Superconductivity in Monatomic Metals," Workshop on Ab-initio Approaches to Electron-Phonon Coupling and Superconductivity, San- Sebastian, Spain, (May 2007).
144."Realistic Tight-Binding Methodologies," International Symposium on Metastable and Nano Materials, Corfu, Greece, (August 2007).
145."Realistic Tight-Binding Methodologies," NIST, (September 2007).
146."The NRL Tight-binding Method," International Conference on Computational Materials Science, Cocoyoc, Mexico, (February 2008).
147."First-principles, Tight-binding, and Embedded-atom Calculations

in the Pd-H System," XVII International Materials Research Congress," Cancun, (August 2008).
148. "Tight-binding Hamiltonians for Fe-based Pnictides and Other Systems," Virginia Commonwealth University, (April 2010).
149. "Tight-binding Hamiltonians from Solids to Molecules", Conference on Wave Propagation, Crete, Jun 2011.
150. "Quantum Mechanics Exploration of Graphene-like Systems to Model Magnetic Resonators", AVS 58th Intern. Symposium, Nashville, TN Nov 2011.
151. "Tight-binding Method Applied to Magnetic Systems", 4th Workshop on Current Trends in Molecular and Nanoscale Magnetism, Ouranoupolis, Greece, Jun 2012.
152. "Electron-Phonon Coupling in Pnictides", Workshop on Novel Materials, Univ. Cal Davis Jun 2012.
153. "Applications of the Gaspari-Gyorffy Theory", Conference on Superconductivity, Magnetism, and Electron Correlations, Bristol, England, Jul 2014.
154. "High-temperature superconductivity at high pressures for H3SixP(1-x), H3PxS(1-x) and H3ClxS(1-x)", International Workshop: Towards Room Temperature Superconductivity: Hydrides and more, Rome, Italy, May 2016.
155. "The electron-phonon coupling in light-element hydrides" , Second International Workshop : Towards Room Temperature Superconductivity: Superhydrides and More, Chapman University, Orange, CA, May 2017.