

Resume

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Citizenship: United States of America

Education:

Bachelor of Science in Physics, Calcutta University , India , 1967

Bachelor of Technology in Radio-Physics & Electronics, Calcutta University ,
India , 1969

Master of Science in Physics, Oklahoma State University , Stillwater , Oklahoma ,
1973

Master of Science in Mathematics, Texas Tech University , Lubbock , Texas ,
1975

Doctor of Philosophy in Physics, Texas Tech University , Lubbock , Texas , 1977

Academic Employments:

1971-1973 Graduate Teaching Assistant, Department of
Physics, Oklahoma State University

1973-1974 Part-Time Instructor, Department of Mathematics, Texas Tech
University

- 1974-1978 Instructor, Department of Physics, Texas Tech University
- 1977-1978 Research Assistant, Department of Mathematics, Texas Tech
University
- 1978-1979 Visiting Assistant Professor, Department of Physics, Texas
Tech
University
- 1979-1981 Postdoctoral Research Associate, Quantum Theory Project,
Departments of Physics and Chemistry, University of Florida
- 1981-1982 Assistant Professor, Department of Physics, Michigan
Technological University
- 1979-1986 Staff Member, Institute for Numerical Transport Theory,
Department of Mathematics, Texas Tech University
- 1982-1984 Visiting Assistant Professor, Department of Physics, University
of Texas at Arlington
- 1984-1988 Assistant Professor, Department of Physics, University of
Texas

at Arlington

- Summer, 1987 Visiting Research Fellow, University of East Anglia , Norwich ,
United Kingdom
- 1988 - 1992 Associate Professor, Department of Physics, University of
Texas at Arlington
- Fall, 1990 Guest Professor, Institute for Technical Electrochemistry,
Technical University of Vienna , Austria
- March, 1991 Visiting Research Fellow, Department of Theoretical
Chemistry,
Oxford University , United Kingdom
- 1992-cont. Professor, Department of Physics, University of Texas at
Arlington
- August, 1998 Visiting Research Chemist, Department of Chemistry,
Princeton
University, Princeton , New Jersey
- Oct.-Nov. 1998 Visiting Scientist, Los Alamos National Laboratory, Los Alamos
,
New Mexico

Dec. 1998-1999 Consultant, Los Alamos National Laboratory, Los Alamos ,
New

Mexico

Dec. 1998-Jan. Visiting Research Chemist, Department of Chemistry,
Princeton

1999 University, Princeton , New Jersey

July-Aug. 1999 Visiting Research Fellow, Department of Chemistry, Princeton
University, Princeton , New Jersey .

Research Interests:

Electronic Structures of the Actinides

Computational Electronic Structure Theory of Solids and Surfaces

Computational Studies of Nanostructures and Clusters

Computational Electron Transport Theory

Refereed Research Publications:

1. *Invited Paper*: "Model-Independent Determination of Nuclear Radii," (with Y. N. Kim and S. Wald), Proceedings of the Second Nuclear Conference of the European Physical Society, Vol. II, 34-52, Cracow , Poland (1976).
2. "On the Effectiveness of the Inverse Riccati Transformation in the Matrix Case," (with P. Nelson and G. M. Wing), Journal of Mathematical Analysis and Applications, **65**, 201-210 (1978).
3. "A Theoretical Result on the Effectiveness of the Addition Formulae for Two-Point Boundary Systems," (with P. Nelson and G. M. Wing), Journal of Mathematical Analysis and Applications, **67**, 392-399 (1979).
4. "A Unique Parameterization for the Transition Potential in Muonic X-Rays," (with S. Wald and Y. N. Kim), Zeitschrift fur Physik, **289A**, 391-394 (1979).
5. "Exact Calculations for Penetrability and the Prediction of the Spontaneous Fission Half-Lives of Superheavy Elements," (with S. Wald and M. A. K. Lodhi), Proceedings of International Conference on Superheavy Elements, Pergamon Press , New York , 467-478, (1979).
6. "Possible Muonic Transitions and X-Ray Spectra from Superheavy Elements," (with S. wald and M. A. K. Lodhi), Proceedings of International Conference on Superheavy Elements, Pergamon Press , New York , 442-450 (1979).

7. "An Automatic Error-Control Technique for Computations of Eigenlengths," (with P. Nelson), Journal of Computational Physics, **37**, 388-398 (1980).
8. "More Corrections to the Sixth Order Anomalous Magnetic Moment of the Muon", (with M. L. Laursen and M. A. Samuel), Zeitschrift fur Physik, **6C**, 3-6 (1980).
9. "Lattice Constant at the Insulator-Metal Transition of Crystalline Xenon," (with S. B. Trickey, R. S. Weidman and A. B. Kunz), Physical Review Letters, **45**, 933-935 (1980).
10. "Oscillation and Comparison Theorems for $y''(x) + \lambda a(x)y(x) = 0$," (with R. M. Anderson), Journal of Mathematical Analysis and Applications, **83**, 100-109 (1981).
11. "Adequacy of Local Exchange Excitation Hamiltonians in Insulators," (with S. B. Trickey and J. P. Worth), Physica Status Solidi, **106**, 613-620 (1981).
12. "Augmented Plane Wave to Gaussian Orbital Conversion Procedure: One Electron States and Compton Profiles of FCC Neon," (with S. B. Trickey), Physical Review B, **24**, 1751-1760 (1981).
13. "BCC-FCC Allotropy, F-Bands, and Metallization in Xenon and Krypton," (with S. B. Trickey and A. B. Kunz), Solid State Communications, **41**, 351-353 (1982).
14. "GCM Treatment of Some Model Periodic Systems," (with L. R. Kauder and S. B. Trickey), International Journal of Quantum Chemistry, **23**, 1355-1361 (1983).

15. "Computation of Electron Transport in Layered Media by Invariant Imbedding," (with P. Nelson and J. C. Garth), Advances in Reactor Computations, American Nuclear Society, **Vol. II**, 623-633 (1983).
16. "Optical Absorption of Solid Xenon at High Pressure," (with S. B. Trickey and A. B. Kunz), Physica Status Solidi, **121**, K47-50 (1984).
17. "Central Depression in ^4He Charge Density and Form Factor," (with M. A. K. Lodhi), Proceedings of International Conference on Nuclear Physics, (Tipografia Compositori, Bologna), **Vol. I**, 321 (1984).
18. "The Electronic Structure of Nitromethane: A Multi-Configurational Self-Consistent-Field Study," (with D. S. Marynick, J. L. Fry and D. A. Kleier), Journal of Molecular Structure, **108**, 45-48 (1984).
19. "Computational Study of the Upwind Finite-Difference Method," (with P. Nelson and D. L. Seth), Transactions of the American Nuclear Society, **46**, 436-438 (1984).
20. "A Configuration Interaction Study of Small Lithium Clusters," (with J. L. Fry and C. W. Myles), Journal of Physics B, **18**, 381-386 (1985).
21. "Electronic Structure Calculations on R-NO₂ Species, R=H, CH₃, NH₂, HO and F," (with D. S. Marynick and J. L. Fry), Chemical Physics Letters, **116**, 429-433 (1985).
22. "Surface Effects in Cluster Calculations of Energy Profiles of Mu in Diamond," (with S. Estreicher , J. L. Fry and D. S. Marynick), Physical Review Letters, **55**, 1976-1978 (1985).

23. "A Study of Positron Diffusion and Annihilation in Gases," (with S. R. Kafle, J. L. Fry and S. C. Sharma), Proceedings of Seventh International Conference on Positron Annihilation, World Scientific Publishing, 359-361 (1986).
24. "Minimal Basis-Set SCF-MO Calculations on Aggregates of Lithium and Beryllium Atoms," Journal of Physics B, **19**, 1253-1259 (1986).
25. "Electron Transport in Layered Media by Invariant Imbedding," (with P. Nelson and J. C. Garth), Proceedings of the Conference on Integral Methods in Science and Engineering, Hemisphere Publishing, 37-53 (1986).
26. "Interstitial Hydrogen in Diamond: A Detailed Hartree-Fock Analysis," (with S. Estreicher , J. L. Fry and D. S. Marynick), Physical Review B, **34**, 6071-6079 (1986).
27. "A Hartree-Fock Study of Carbon Clusters," Journal of Physics B, **20**, 5233-5239 (1987).
28. "A Theoretical Study of Carbon Clusters: Equilibrium Geometries and Electronic Structures of C_n " (with L. S. Ott), Proceedings of the NATO Advanced Workshop and International Symposium on the Physics and Chemistry of Small Clusters, Plenum Publishing, New York, 95-101 (1987).
29. "An *Ab Initio* Study of the Interaction of Atomic Hydrogen with Lithium Clusters," (with A. S. Hira and J. L. Fry), Proceedings of the NATO Advanced Workshop and International Symposium on the Physics and Chemistry of Small Clusters, Plenum Publishing, New York , 413-419 (1987).
30. "Response to Comment on Surface Effects in Cluster Calculations of Energy Profiles of Mu in Diamond," (with S. Estreicher , J. L. Fry and D. S. Marynick), Physical Review Letters, **57**, 3301 (1987).

31. "Many Body Perturbation Theory Applied to Hydrogen Interaction with Lithium Clusters," (with A. S. Hira), Physical Review B, **37**, 9943-9950 (1988).
32. "Many Body Perturbation Theory Applied to Small Germanium Clusters," (with M. S. Islam), Chemical Physics Letters, **153**, 496-502 (1988).
33. "A Note on the Bhatia Theory of Liquid NaSn Alloys," (with W. H. Young), Physics and Chemistry of Liquids, **19**, 7-9 (1989).
34. "A Hartree-Fock Study of Ionized Carbon Clusters," (with M. S. Islam), Journal of Physics B, **22**, 2071-2079 (1989).
35. "*Ab Initio* Study of H Chemisorption on Li Clusters in FCC(100) Symmetry," (with A. S. Hira), Physical Review B, **40**, 3507-3513 (1989).
36. "*Ab Initio* Many Body Perturbation Theoretic Study of Small Sodium Clusters," Solid State Communications, **71**, 311-316 (1989).
37. "Short Range Form of the Charge Distribution of ^4He and Its Charge Form Factor," (with M. A. K. Lodhi and C. Yalcin), IL Nuovo Cimento, **101A**, 155-162 (1989).
38. "*Ab Initio* Many Body Perturbation Theoretic Study of Sodium Cationic Clusters," Solid State Communications, **72**, 1051-1056 (1989).
39. "*Ab Initio* Many Body Perturbation Theoretic Study of Small Potassium Clusters," (with S. D. Altekar), Physical Review B, **42**, 1444-1447 (1990).

40. "An *Ab Initio* Study of Neutral K_nNa and Cationic K_nNa^+ Clusters," (with S. P. Berry), Journal of Physics B, **23**, 2365-2377 (1990).
41. "An *Ab Initio* Study of Small Potassium Cationic Clusters," (with S. D. Altekar), Physica Status Solidi, **161**, 463-472 (1990).
42. "A Correlation Study of H Interaction with Li Clusters in BCC(111) Symmetry," (with A. S. Hira), Surface Science, **234**, 397-411 (1990).
43. "A Correlation Study of Chemisorption of Atomic Oxygen on Li BCC Clusters," (with A. S. Hira), Journal of Physics B, **24**, 881-896 (1991).
44. "An *Ab Initio* Study of H Chemisorption on Li Clusters in FCC(110) and FCC(111) Symmetries," (with A. S. Hira), Surface Science, **249**, 199-212 (1991).
45. "On the Existence and Stability of Small K_nMg Clusters," (with S. D. Altekar), Journal of Physics: Condensed Matter **3**, 8319-8326 (1991).
46. "A Correlation Study of Large Potassium Cationic Clusters," (with K. M. Kanal and I. A. Howard), Physica Status Solidi, **167**, 465-475 (1991).
47. "Lithium Atom Chemisorption on Silicon Clusters," (with S. N. Ekpenuma), Surface Science, **257**, L659-L664 (1991).
48. "Isomer Shifts and Electric Field Gradients in Y ($Fe_{1-x}Al_x$)," (with P. Blaha and K. Schwarz), Journal of Magnetism and Magnetic Materials, **104**, 683-684 (1992).

49. "Adsorption of Monatomic Hydrogen in Icosahedral Borides," (with I. A. Howard), Physical Review B, **45**, 3680-3684 (1992).
50. "Structure and Binding in Small Neutral and Cationic Boron Clusters," (with I. A. Howard and K. M. Kanal), Physical Review B, **45**, 14247-14255 (1992).
51. "A Correlation Study of Large Potassium Neutral Clusters," (with K. M. Kanal and I. A. Howard), Physica Status Solidi, **171**, 131-140 (1992).
52. "Correlation Study of Sodium Atom Chemisorption on Silicon Surface," (with S. N. Ekpenuma), Journal of Physics: Condensed Matter, **4**, 5077-5086 (1992).
53. "A Correlation Study of Large Neutral and Singly Ionized Carbon Clusters," (with M. S. Islam), Journal of Physics: Condensed Matter, **4**, 4101-4114 (1992).
54. "Stabilities of Adsorption Sites and Charge Transfers at the K/Si (001) Surface," (with S. N. Ekpenuma), Physical Review B, **46**, 16163-16166 (1992).
55. "A Computational Study of the Discretization Error in the Solution of the Spencer-Lewis Equation by Doubling Applied to the Upwind Finite Difference Approximation," (with P. Nelson and D. L. Seth), Journal of Computational Physics, **103**, 370-381 (1992).
56. "A Note on 2-D Electron Transport Using Discrete Ordinates," (with R. P. Datta, A. S. Hira and B. R. Wienke), Supercomputer, **9**, 15-21 (1992).

57. "A Hartree-Fock Study of Small Carbon Cluster Anions," (with B. K. Rao), Physics and Chemistry of Finite Systems: From Clusters to Crystals, Kluwer Academic Publishing, 645-650 (1992).
58. "On the Parallelization of a S_n Transport Algorithm on a Cray Y-MP," (with S. D. Altekar and B. R. Wienke), Parallel Computing, **19**, 823-834 (1993).
59. "On the Interaction of a Sodium Atom with the Silicon (111) Surface," (with M. Mahapatra and A. S. Hira), Journal of Physics: Condensed Matter **5**, 6543-6554 (1993).
60. "A Discrete-Ordinates Study of Two Dimensional Electron Transport," (with R. P. Datta and B. R. Wienke), Journal of Physics D: Applied Physics, **26**, 1077-1083 (1993).
61. "Stability of Clusters in Two Dimensions," (with B. K. Rao and P. Jena), Physical Review B, **42**, 14702-14705 (1993).
62. "A Spatial Characteristic Scheme for Multigroup Discrete Ordinates Electron Transport in Two Dimensions," (with R. P. Datta), Physica Status Solidi, **180**, 85-95 (1993).
63. "Three Particle Correlation Function and Structural Theories of Dense Metallic Liquids," (with K. I. Golden and N. H. March), Molecular Physics, **80**, 915-924 (1993).
64. "Correlation Study of Sodium Atom Chemisorption on the GaAs(110) Surface," (with K. M. Song and D. C. Khan), Physical Review B, **49**, 1818-1826 (1994).

65. "A Diffraction Study of the Structure of Liquid Potassium Near Freezing and Density Functional Theory of Pair Potentials," (with M. W. Johnson, N. H. March and F. Perrot), Philosophical Magazine, **69**, 965-977 (1994).
66. "A Cluster Study of the Stabilities of Adsorption Sites and Charge Transfers at the Na/Si (100) Surface," (with P. C. Lin and A. S. Hira), Physica Status Solidi, **182**, 331-345 (1994).
67. "On the Electronic Structures of GaAs Clusters," (with K. M. Song and P. Khowash), Journal of Physics B, **27**, 1637-1647 (1994).
68. "Exploiting Parallelism in a S_n Transport Algorithm : An Angular Approach." (with S. D. Altekar), Parallel Algorithms and Applications, **4**, 317-328 (1994).
69. "An *Ab Initio* Study of Potassium Chemisorption on GaAs (110) Surface," (with K. M. Song), Journal of Physics: Condensed Matter, **6**, 9571-9583 (1994).
70. "An *Ab Initio* Study of Cesium Chemisorption on the GaAs(110) Surface," (with K. M. Song), Physical Review B, **50**, 14255-14266 (1994).
71. "A Computational Model for Electron Backscattering in Electron Dosimetry," (with T. Kellogg), Medical Physics, **22**, 25-30 (1995).
72. "Geometries and Electronic Structures of Negatively Charged Carbon Clusters," (with B. K. Rao), Zeitschrift fur Physik D, **33**, 197-201 (1995).
73. "Interaction Sites of a Na^+ Ion and a Na Atom with a C_{60} Molecule," (with A. S. Hira), Physical Review A, **52**, 141-148 (1995).

74. "Diatomic Heteronuclear Iron-Metal(3d) Molecule Clusters and their Electronic Structures (with H. J. Choi and A. M. Lemos), Journal of the Korean Physical Society, **28**, 796-798 (1995).
75. "On the Choice of Basis Sets for the Study of Chemisorption of Hydrogen on Aluminum," (with P. C. Lin, J. Niu and B. K. Rao), Proceedings of the International Symposium of the Science and Technology of Atomically Engineered Materials , World Scientific Publishing, 275-279 (1996).
76. "Anomalous Spectroscopy of Li_4^- Cluster," (with B. K. Rao and P. Jena), Physical Review Letters, **76**, 2878-2881(1996).
77. "A Computational Model for Coupled Electron-Photon Transport in Two Dimensions," (with R. P. Datta, S. D. Altekhar and J. E. Morel), Physical Review E, **53**, 6514-6522 (1996).
78. "Interactions of the Na_2 Dimer with a C_{60} Molecule," (with A. S. Hira), Physical Review A, **54**, 2205-2215 (1996).
79. "A Cluster Study of Rb Atom Chemisorption on GaAs (110) Surface," (with K. M. Song), Journal of Physics: Condensed Matter, **8**, 6617-6627 (1996).
80. "Geometries and Energies of Small Aluminum Clusters in FCC Symmetry," (with B. K. Rao), Journal of Physics : Condensed Matter, **9**, 2859-2868 (1997).
81. "A Correlation Study of Boron Dimers and Trimers," (with I. A. Howard), Zeitschrift fur Physik D, **42**, 299-301 (1997).

82. "Force Fields in Liquid and Solid Cu Metal: Relation between Quantum Chemical and Density Functional Treatments," (with N. H. March), Physics and Chemistry of Liquids, **36**, 207-214 (1998).
83. "A Density Functional Study of Small Neutral and Cationic Vanadium Clusters V_n and V_n^+ ($n=2-9$)," (with X. Wu), Journal of Chemical Physics, **110**, 2437-2445 (1999).
84. " Si_n Clusters: Surface Energy Considerations for Large n and All-Electron Hartree-Fock Calculations for $n=45$," (with N. H. March, D. J. Klein and X. Wu), International Journal of Quantum Chemistry, **75**, 829-838 (1999).
85. "A Density Functional Cluster Study of K Adsorption on GaAs (110) Surface," (with M. Panda), Journal of Vacuum Science and Technology A, **17**, 2647-2654 (1999).
86. "An *Ab Initio* Cluster Study of Chemisorption of Atomic Cs on Ga-Rich GaAs (100) (2x1), (2x2) and (4x2) Surfaces," (with R. Schailey), Journal of Chemical Physics, **111**, 8628-8638 (1999).
87. "Possible Existence of the Plutonium Dimer," (with E. Archibong), Physical Review A, **60**, 5105-5107 (1999).
88. "Relation between Vacancy Properties and Surface Energies in Three Noble or Transition Metals (with N. H. March), Journal of Physics and Chemistry of Solids, **61**, 827-828 (2000).
89. "All-Electron Density Functional Theory Calculations of the Zero-Pressure Properties of Plutonium Dioxide," (with J. C. Boettger), AIP Conference Proceedings 532, Plutonium Futures-The Science, edited by K. K. S. Pillay and K. C. Kim , 532-422 (2000).

90. "An *Ab Initio* Study of PuO₂ and PuN₂," (with E. Archibong), Journal of Molecular Structure (TheoChem), **530**, 165-170 (2000).
91. "All Electron LCGTO Calculations for Uranium Dioxide," (with J. C. Boettger), International Journal of Quantum Chemistry, **80**, 824-830 (2000).
92. "A Hybrid Density Functional Cluster Study of the Bulk and Surface Electronic Structures of Plutonium Monoxide," (with X. Wu), Physica B, **293**, 362-375 (2001).
93. "A Hybrid Density Functional Cluster Study of the Bulk and Surface Electronic Structures of Plutonium Dioxide," (with X. Wu), Physica B, **301**, 359-369 (2001).
94. "A Density Functional Study of Plutonium Dioxide," (with X. Wu), European Physical Journal B, **19**, 343-351 (2001).
95. "A Cluster Approach to Hydrogen Chemisorption on GaAs (100) Surface," (with R. Schailey), Computational Materials Science, **22**, 169-179 (2001).
96. "A Density Functional Study of Water Adsorption on PuO₂ (110) Surface," (with X. Wu), Physical Review B, **65**, 085403 (2002).
97. "On the Electronic Structures of Gold Tetramer Clusters," Computational Materials Science, **25**, 279-284 (2002).

98. "An All-Electron LCGTO Study of Square and Hexagonal Plutonium Monolayers," (with J. C. Boettger), European Physical Journal B, 27, 429-433 (2002).
99. "Fully Relativistic Density Functional Calculations on Hydroxylated Actinide Oxide Surfaces," (with J. C. Boettger), International Journal of Quantum Chemistry, 90, 1470 – 1477 (2002).
100. "A Correlation Study of Small Silver Clusters," (with M. N. Huda), European Physical Journal D, 22, 217-227 (2003).
101. "Electronic Structures and Magic Numbers of Small Silver Clusters: A Many Body Perturbation Theoretic Study," (with M. N. Huda), Physical Review A, 67, 013201-1-13 (2003).
102. "Quantum Size Effects in Hexagonal Plutonium Layers," (with J. C. Boettger), AIP Conference Proceedings, 673, 198-200 (2003).
103. "Carbon Dimer in Silicon Cage: A Class of Highly Stable Silicon Carbide Clusters," (with M. N. Huda), Physical Review A (Rapid Communications), 69, 011201-4 (2004).
104. "Carbon Dimer in Silicon Cage: A Class of Highly Stable Silicon Carbide Clusters," (with M. N. Huda), Virtual Journal of Nanoscale Science and Technology, Feb. 9 (2004).
105. "A First-Principles Electronic Structure Study of Quantum Size Effects in (111) Films of δ -Plutonium," (with J. C. Boettger), Physical Review B, 70, 085418-1-6 (2004).

106. "Electronic Structure and Bonding of Oxygen on Plutonium Layers," (with M. N. Huda), European Physical Journal B, **40**, 337-346 (2004).
107. "A Density Functional Study of Atomic Hydrogen Adsorption on Plutonium Layers," (with M. N. Huda), Physica B, **352**, 5-17 (2004).
108. "Novel Silicon-Carbon Fullerene-Like Cages: A Class of sp^2 - sp^3 Covalent-Ionic Hybridized Nanosystems", (with M. N. Huda), European Physical Journal D, **31**, 63-68 (2004).
109. "Density Matrix Force-Balance Equation Applied to He, Be, and Ne atoms and to Almost-Spherical Methane-Like Molecules," (with I. A. Howard, N. H. March, F. Bartha, and M.-L. Zhang), International Journal of Quantum Chemistry, **100**, 155-165 (2004).
110. "A Density Functional Study of the Structure and Energetics of Small Hetero-Atomic Silicon-Carbon Nanoclusters," (with P. Pradhan), Journal of Molecular Structure: THEOCHEM, **716**, 109 -130 (2005).
111. "A Density Functional Study of O₂ Adsorption on the (100) Surface of γ - Uranium," (with M. N. Huda), International Journal of Quantum Chemistry, **102**, 98-105 (2005).
112. "A Density Functional Study of Molecular Oxygen Adsorption and Reaction Barrier on Pu (100) Surface," (with M. N. Huda), European Physical Journal B, **43**, 131-141 (2005).
113. "An *Ab Initio* Study on the Use of Ag₂- for Catalytic Oxidation of CO," (with P. Dholabhai and X. Wu), Journal of Molecular Structure: THEOCHEM, **723**, 139-145 (2005).

114. "A Cluster Study of Aluminum Adsorption on Ga-Rich GaAs (100) (2x1) and β (4x2) Surfaces," (with M. L. Mayo), European Physical Journal D, **33**, 413-420 (2005).
115. "A Full-Potential-Linearized-Augmented-Plane-Wave Electronic Structure Study of δ - Plutonium and the (001) Surface," (with X. Wu), Physical Review B, **72**, 045115-1-9 (2005).
116. "An *Ab Initio* Study of H₂ Interaction with the Pu (100) Surface," (with M. N. Huda), Physica B, **366**, 95-109 (2005).
117. "Molecular Hydrogen Adsorption and Dissociation on the Pu (111) Surface," (with M. N. Huda), Physical Review B, **72**, 085101-1-11 (2005).
118. "An *Ab Initio* Study of Molecular Oxygen Adsorption on Pu (111) Surface," (with M. N. Huda), International Journal of Quantum Chemistry, **105**, 280-291 (2005).
119. "Relativistic LCGTO-FF Calculations of Quantum Size Effects in Plutonium Films," (with J. C. Boettger), International Journal of Quantum Chemistry, **105**, 564-570 (2005).
120. "Quantum Size Effects in δ - Pu (110) Films," (with H. R. Gong), European Physical Journal B, **48**, 409-416 (2005).
121. "Silicon-Carbon Fullerene-Like Nanostructures : An *Ab Initio* Study on the Stability of Si₆₀ C_{2n} (n = 1, 2) Clusters," (with A. Srinivasan and M. N. Huda), Physical Review A, **72**, 063201-1-10 (2005).

122. "An *Ab Initio* Study of Charge State Effects on the Use of Ag_2^+ and Ag_2 for Catalytic Oxidation of CO," (with P. Dholabhai), Journal of Theoretical and Computational Chemistry, **4**, 1075-1091 (2005).
123. "Novel Silicon-Carbon Fullerene-Like Nanostructures : An *Ab Initio* Study on the Stability of Si_{54}C_6 and Si_{60}C_6 Clusters," (with A. Srinivasan), Journal of Nanoscience and Nanotechnology, **6**, 43-53 (2006). *Cover page has a copy of one of our figures.*
124. "A Hybrid Density Functional Study of Armchair Si and Ge Nanotubes," (with P. Pradhan), Journal of Computational and Theoretical Nanoscience, **3**, 128-133 (2006).
125. "An *Ab Initio* Study on the Electronic and Geometric Structures of Si_mC_n^+ Cationic Nanoclusters," (with P. Pradhan), European Physical Journal D, **37**, 393-407 (2006).
126. "5f Delocalization of Bulk FCC Americium and the (111) Surface : A FP-LAPW
Electronic Structure Study," (with D. Gao), Actinides 2005 – Basic Science, Applications and Technology, MRS Symposium Proceedings, **803**, 39-44 (2006).
127. "A First-Principles Study of the (111), (001), and (110) Surfaces of δ – Pu," (with H. R. Gong), Actinides 2005 – Basic Science, Applications and Technology, MRS Symposium Proceedings, **803**, 44-50 (2006).
128. "The 5f Localization – Delocalization in Square and Hexagonal Americium Monolayers – A FP-LAPW Electronic Structure Study," (with D. Gao), European Physical Journal B, **50**, 497-503 (2006).

129. "A Fully-Relativistic Full-Potential-Linearized-Augmented-Plane-Wave Study of the (111) Surface of δ - Pu," (with H. R. Gong), Surface Science, **600**, 2231-2241 (2006).
130. "Silicon-Carbide Nano Clusters: A Pathway to Future Nano – Electronics," (with M. N. Huda), *Review Article*, Journal of Computational and Theoretical Nanoscience, **3**, 315-341 (2006).
131. "A Density Functional Theoretic Study of Novel Silicon-Carbon Fullerene-Like Nanostructures: $\text{Si}_{40}\text{C}_{20}$, $\text{Si}_{60}\text{C}_{20}$, $\text{Si}_{36}\text{C}_{24}$, and $\text{Si}_{60}\text{C}_{24}$," (with A Srinivasan and M. N. Huda), European Physical Journal D, **39**, 227-236 (2006).
132. "On the Convergence of the Electronic Structure Properties of the FCC Americium (001) Surface," (with D. Gao), Surface Science, **600**, 4941-4952 (2006).
133. "A Full Potential–Linearized Augmented Plane Wave (FP-LAPW) Study of Atomic Carbon, Nitrogen, and Oxygen Chemisorption on the (100) Surface of δ -Pu," (with R. Atta-Fynn), Physica B, **392**, 112 - 126(2007).
134. "A Density Functional Study of Atomic Oxygen and Carbon Adsorptions on (100) Surface of γ – Uranium," (with P. Dholabhai), Physica Scripta, **75**, 506-514 (2007).
135. "Quantum Size Effects in the (0001) Surface of Double Hexagonal Close Packed Americium (with D. Gao), European Physical Journal B, **55**, 13-22 (2007).
136. "An *Ab Initio* Full Potential Fully Relativistic Study of Atomic Carbon, Nitrogen, and Oxygen Chemisorption on the (111) Surface of δ -Pu," (with R. Atta-Fynn), Physical Review B, **75** , 195112-1-13 (2007).

137. "An *Ab Initio* Computational Study of Atomic Adsorption on GaAs Surfaces Modeled by Nanoclusters," (with M. L. Mayo), Journal of Computational and Theoretical Nanoscience, **4**, 443-452 (2007).
138. "Silicon Carbide Nanostructures to Nanotubes," (with M. N. Huda and L. Kleinman), Journal of Computational and Theoretical Nanoscience, **4**, 739-744 (2007); *Cover page has a copy of one of our figures.*
139. "A First-Principles Electronic Structure Study of the High-Symmetry Surfaces of FCC Americium," (with D. Gao), Journal of Alloys and Compounds, **444-445**, 184-190 (2007).
140. "A Density Functional Study of Carbon Monoxide Adsorption on the (100) Surface of γ -Uranium," (with P. Dholabhai), Journal of Alloys and Compounds, **444-445**, 356-362 (2007).
141. "A Fully Relativistic Density Functional Study of the Actinide Nitrides," (with R. Atta-Fynn), Physical Review B, **76**, 115101-1-12 (2007).
142. "Relaxation of the (111) Surface of δ - Pu and Effects on Atomic Adsorption - An *Ab Initio* Study," (with R. Atta-Fynn), Physica B, **400**, 307-316 (2007).
143. "A Hybrid Density Functional Study of Zigzag Silicon Carbide Nanotubes," (with K. Alam), Nanotechnology, **18**, 495706-1-10 (2007).
144. "First Principles Calculations of Localization of *5f* Electrons in Bulk Alpha-Plutonium," (with H. R. Gong), Journal of the Physical Society of Japan, **76**, 114701-1-4 (2007).

145. "A Relativistic Density Functional Study of FCC Americium and the (111) Surface," (with D. Gao), Physical Review B, **77**, 035123-1-9 (2008).
146. "Hybrid Density Functional Study of Armchair Silicon Carbide Nanotubes," (with K. Alam), Physical Review B, **77**, 035436-1-10 (2008).
147. "Hybrid Density Functional Study of Armchair Silicon Carbide Nanotubes," (with K. Alam), Virtual Journal of Nanoscale Science and Technology, February 11 (2008).
148. "Atomic Adsorption on the (020) Surface of α - Pu - A Density Functional Study," (with R. Atta-Fynn), Physical Review B, **77**, 085105-1-11(2008).
149. "A Density Functional Study of Atomic Hydrogen and Oxygen Chemisorption on the Relaxed (0001) Surface of Double Hexagonal Close Packed Americium," (with P. Dholabhai and R. Atta-Fynn), European Physical Journal B, **61**, 261-270 (2008).
150. "A Hybrid Density Functional Study of Zigzag and Chiral Silicon Nanotubes," (with S. Rathi), Journal of Computational and Theoretical Nanoscience, **5**, 464-475 (2008).
151. "Evolution of SiC NanoCluster from Carbon Fullerene : A Density Functional Theoretic Study," (with M. N. Huda), Chemical Physics Letters, **457**, 124-129
(2008).
152. "On the Electronic and Geometric Structures of Armchair GeC Nanotubes - A Hybrid Density Functional Study," (with S. Rathi), Nanotechnology, **19**, 335706 - 335716 (2008).

153. "An *Ab Initio* Study of Molecular Hydrogen Interaction with SiC Nanotube – A Precursor to Hydrogen Storage," (with S. Mukherjee), Journal of Computational and Theoretical Nanoscience, **5**, 1210-1219 (2008).
154. "On the Existence and Stability of Single Walled SiGe Nanotubes," (with S. Rathi), Chemical Physics Letters, **466**, 79-83 (2008)..
155. "An *Ab Initio* Study of the Adsorption and Dissociation of Molecular Oxygen on the (0001) Surface of Double Hexagonal Close Packed Americium," (with P. Dholabhai and R. Atta-Fynn), Physica B, **403**, 4269-4280 (2008).
156. "A First Principles Study of the Interactions of Fe Atom with Single Walled Zigzag SiC Nanotubes," (with K. Alam), Journal of Computational and Theoretical Nanoscience, **6**, 16-29 (2009).
157. "Does Hybrid Density Functional Theory Predict a Non-Magnetic Ground State for δ – Pu?," (with R. Atta-Fynn), Europhysics Letters, **85**, 27008-p1-p6 (2009).
158. "Adsorption and Dissociation of Molecular Hydrogen on the (0001) Surface of Double Hexagonal Close Packed Americium," (with P. P. Dholabhai), European Physical Journal B, **67**, 183-192 (2009).
159. "A Relativistic DFT Study of Water Adsorption on δ – Pu (111) Surface," (with R. Atta-Fynn), Chemical Physics Letters, **470**, 233-239 (2009).
160. "Adsorption and Dissociation of Water on the (0001) Surface of Double Hexagonal Close Packed Americium," (with P. Dholabhai), Physica Status Solidi B, **246**, 1225-1237 (2009).

- 161.** "A First Principles Study of the Adsorption and Dissociation of CO₂ on the δ -Pu (111) Surface," (with R. Atta-Fynn), European Physical Journal B, **70**, 171-184 (2009)..
- 162.** "Interactions of Fe Atom with Single Wall Armchair SiC Nanotubes : An *Ab Initio* Study," (with K. Alam), Journal of Nanoparticle Research, **11**, 1405-1420 (2009).
- 163.** "Interplay between Spin Polarization, Orbital Polarization, and Spin-Orbit Coupling in Actinides from Pa to Cm," (with F. Islam), Journal of Computational and Theoretical Nanoscience, **6**, 1458-1467 (2009).
- 164.** "Probing the *5f* Electrons in Am-I by Hybrid Density Functional Theory," (with R. Atta-Fynn), Chemical Physics Letters, **482**, 223-227 (2009).
- 165.** "A Computational Study of Endohedral and Exohedral Complexes of Molecular Hydrogen with Single Wall (3,3) to (6,6) Armchair Silicon Carbide Nanotubes," (with S. Mukherjee), Journal of Computational and Theoretical Nanoscience, **7**, 1518-1530 (2010).
- 166.** "A LDA+U Study of the Photoemission Spectra of the Double Hexagonal Close Packed Phases of Am and Cm," (with F. Islam) Solid State Communications, **150**, 938-942 (2010).
- 167.** "On the Magnetic and Thermodynamic Properties of Americium II – A Hybrid Density Functional Theoretic Study," (with J. Wang and Li Ma), Physics Letters A, **374**, 4704 – 4712 (2010).

168. "A Hybrid DFT Description of the (0001) Surface of Americium –I (with R. Atta-Fynn), European Physical Journal B, **78**, 13-22 (2010).
169. "Atomic Hydrogen Adsorption on the (020) Surface of α – Pu – A Computational Study," (with F. Islam), Physica Status Solidi B, **248**, 193-202 (2011).
170. "On the Existence and Stability of Double-Walled Armchair Silicon Carbide Nanotubes," (with K. Adhikari), Solid State Communications, **151**, 430-435 (2011).
171. "Carbon- and Silicon-Capped Silicon Carbide Nanotubes: An *Ab Initio* Study," (with K. Adhikari), Physics Letters A, **375**, 1817-1823 (2011).
172. "A Hybrid Density Functional Theory Study of $\text{PuO}_{2\pm 0.25}$, $\text{UO}_{2\pm 0.25}$, $\text{U}_{0.5}\text{Pu}_{0.5}\text{O}_{2\pm 0.25}$," (with Li Ma), European Physical Journal B, **81**, 103-113 (2011).
173. "Anomalous Dependence of Band Gaps of Binary Nanotubes on Diameters," (with K. Adhikari and M, N, Huda), Journal of Computational and Theoretical Nanoscience, **8**, 1502-1508 (2011).
174. "Adsorption and Dissociation of Molecular Oxygen on α – Pu (020) Surface – A Density Functional Study," (with J. Wang), Physica B, **406**, 3285-3294 (2011).
175. "Co-Adsorptions of Hydrogen Molecules with Single Wall Silicon Carbide Nanotubes: An *Ab Initio* Study," (with S. Mukherjee), Journal of Computational and Theoretical Nanoscience, **8**, 1798-1810 (2011).

176. "Cluster Modeling of Three Types of Armchair Silicon Carbide Nanotubes," (with K. Adhikari), European Physical Journal D, **64**, 353-363 (2011).
177. "A First Principles Study of Water Adsorption on Alpha-Pu (020) Surface," (with J. Wang), Journal of Nuclear Materials, **424**, 138-145 (2012).
178. "Formation Energies and Swelling of Uranium Dioxide by Point Defects," (with Li Ma), Physics Letters, **376**, 1499-1505 (2012)..
179. "An *Ab Initio* Study of Atomic Hydrogen and Oxygen Adsorptions on Armchair Silicon Carbide Nanotubes," (with H. Chen and K. Adhikari), Journal of Computational and Theoretical Nanoscience, accepted for publication.
180. "Quantum Size Effects in the Electronic Structure Properties of γ - U (100) Nanolayers," (with D. Morrison), Journal of Computational and Theoretical Nanoscience, accepted for publication.
181. "Elemental and Mixed Actinide Dioxides: An *Ab Initio* Study" (with Li Ma and R. Atta-Fynn), Journal of Theoretical and Computational Chemistry, accepted for publication.
182. "Silicon Carbide Nanotubes: From Finite Single-Walled to Infinite Multi-Walled," (with K. Adhikari), *Review Article*, Journal of Computational and Theoretical Nanoscience, accepted for publication.
183. "Theoretical Study of SiC Nanostructures: Current Status and a New Theoretical Approach," (with M. N. Huda), *Review Article*, Journal of Computational and Theoretical Nanoscience, accepted for publication.

184. "Growth Behavior and Magnetic Properties of Spherical Uranium Oxide Nanoclusters," (with Li Ma), Journal of Computational and Theoretical Nanoscience, accepted for publication.
185. "Stabilities of Silicon Carbide Nanocones: A Nanocluster Based Study," Journal of Nanoparticle Research, accepted for publication.
186. "Applications and Interpretations of Density Functional Theory with Potential U in Atomic and Molecular Systems," (with M. N. Huda), Journal of Physical Chemistry, submitted for publication.
187. "An *Ab Initio* Study of the Interaction of CO₂ with the α -Pu (020) Surface," (with J. Wang), Chemical Physics Letters, submitted for publication.
188. "Existence and Stability of Co-Axial and Meshed Double-Walled Armchair Silicon Nanotubes," (with H. Chen), Physica E, submitted for publication.
189. "Unusual Bonding Characteristics in a New Type of Single Walled Armchair SiGe Nanotubes," (with P. Wanaguru), Journal of Computational and Theoretical Nanoscience, submitted for publication.

Book Chapters

1. "An *Ab Initio* Study of SiC Nanotubes: Current Status and Future Prospects," (with M. N. Huda and M. M. Al-Jassim), pp. 1-25,

Nanoclusters and Nanostructured Surfaces (Ed. Asok K. Ray, American Scientific Publishers, 2010).

2. "A Hybrid Density Functional Study of GeC and Pure Ge Nanotubes," (with S. J. Rathi), pp. 189-205, *Nanoclusters and Nanostructured Surfaces* (Ed. Asok K. Ray, American Scientific Publishers, 2010).
3. "An *Ab Initio* Study of Molecular Hydrogen Interactions with Silicon Carbide Nanorubes," (with S. Mukherjee), pp. 275-303, *Nanoclusters and Nanostructured Surfaces* (Ed. Asok K. Ray, American Scientific Publishers, 2010).

Research Papers Presented at National and International Conferences

(Contributed and Invited):

1. "Radial Shape of the Nuclear Charge Distribution," (with Y. N. Kim), Texas Academy of Sciences, 1977.
2. "Nuclear Short Range Correlation and Photodisintegration of ^4He ," (with M. A. K. Lodhi), Bulletin of the American Physical Society, **22**, 612 (1977).
3. "Effect of the Short Range Correlation of the Structure of Light Nuclei and Error Resulting from the Approximation," (with M. A. K. Lodhi and Y. W. Yen), Bulletin of the American Physical Society, **23**, 500 (1978).
4. "GCM Treatment of Some Model Periodic Systems," (with L. R. Kauder and S. B. Trickey), Texas Academy of Sciences (1982).

5. "Electron Transport in Layered Media by Invariant Imbedding," (with P. Nelson and J. C. Garth), Bulletin of the American Physical Society, **28**, 428 (1983).

6. "Quantum Size Effects in the Dielectric Function of Small Metallic Particles," (with C. W. Myles), Bulletin of the American Physical Society, **28**, 382 (1983).

7. "Correlation of Exotic Molecules: Using Second Order Many Body Perturbation Theory for Assessment," (with J. T. Waber, A. B. Kunz and R. S. Weidman), Eighth Canadian Symposium on Theoretical Chemistry, Halifax , Nova Scotia , August 6-12 (1983).

8. "Electronic Structure Calculations of Nitrous Acid," (with D. S. Marynick , J. L. Fry and C. J. Liles), Bulletin of the American Physical Society, **29**, 401 (1984).

9. "Positron Diffusion in Molecular Systems," (with S. R. Kafle and J. L. Fry), Bulletin of the American Physical Society, **30**, 404 (1985).

10. "A Comment on the Small Chain Approximation for the Electronic Structure of Polyacetylene," (with D. S. Marynick and J. L. Fry), Bulletin of the American Physical Society, **30**, 524 (1985).

11. "Hartree-Fock Calculation of Electron States in Aggregates of Lithium and Beryllium Atoms," (with J. L. Fry and C. W. Myles), Bulletin of the American Physical Society, **30**, 524 (1985).

12. "Energy Deposition Distribution by Fast Electrons," (with P. Nelson and J. M. Richards), Bulletin of the American Physical Society, **31**, 595 (1986).

13. "Electron Transport in the Quantum Size Effect Regime," (with M. Islam and K. Schwartzman), Bulletin of the American Physical Society, **31**, 595 (1986).
14. "Isotope Shifts in Muonic Atom X-Rays," (with R. M. Marroum), Bulletin of the American Physical Society, **31**, 677 (1986).
15. "Hartree-Fock Calculation of Electron States in Aggregates of Carbon Atoms," Bulletin of the American Physical Society, **31**, 682 (1986).
16. "An *Ab Initio* Study of the Interaction of Atomic Hydrogen with Lithium Clusters," (with A. S. Hira), Poster Presentation, NATO Advanced Workshop and International Symposium on the Physics and Chemistry of Small Clusters, Virginia Commonwealth University , Richmond , Virginia (1986).
17. "A Theoretical Study of Carbon Clusters: Equilibrium Geometries and Electronic Structures of C_n ," (with L. S. Ott), Poster Presentation, NATO Advanced Workshop and International Symposium on the Physics and Chemistry of Small Clusters, Virginia Commonwealth University , Richmond , Virginia (1986).
18. " Monte Carlo Evaluation of Feynman Path Integrals," (with T. E. Cathey), Bulletin of the American Physical Society, **32**, 476 (1987).
19. "Hartree-Fock Calculations of Electron States in Ionized Carbon Clusters," (with M. Islam), Bulletin of the American Physical Society, **32**, 602 (1987).
20. "Chemisorption Studies of the Interactions of a Hydrogen Atom with Lithium Clusters," (with A. S. Hira), Bulletin of the American Physical Society, **32**, 603 (1987).

21. "Hartree-Fock Study of Ionized Carbon Clusters," (with M. Islam), Poster Presentation, Southwest Theoretical Chemistry Conference, Stephenville , Texas (1987).
22. "An *Ab Initio* Study of Li_3 , Li_4 , and Li_5 Clusters in the FCC(100) Symmetry," (with A. S. Hira), Poster Presentation, Southwest Theoretical Chemistry Conference, Stephenville , Texas (1987).
23. "Ionized Carbon Clusters: An *Ab Initio* Point View," (with M. Islam), Bulletin of the American Physical Society, **33**, 789 (1988).
24. "An *Ab Initio* Study of the Interactions of a Hydrogen Atom with Lithium Clusters in FCC(100) Symmetry," (with A. S. Hira), Bulletin of the American Physical Society, **33**, 816 (1988).
25. "An *Ab Initio* Study of Li_n ($n=3-7$) Clusters in FCC(100) Symmetry," (with A. S. Hira), Poster Presentation, Fourth International Symposium on Small Particles and Inorganic Clusters, Aix-En-Provence , France (1988).
26. "A Study of the Discretization Error in the Computational Solution of the Spencer-Lewis Equation," Bulletin of the American Physical Society, **35**, 259 (1990).
27. "Many Body Perturbation Theory Applied to Neutral and Cationic Potassium K_n ($n=2-7$) Clusters," (with S. D. Altekar), Bulletin of the American Physical Society, **35**, 312 (1990).
28. "Chemisorption of Atomic Hydrogen on Lithium Clusters in the BCC (100), (110) and (111) Symmetries," (with A. S. Hira), Bulletin of the American Physical Society, **35**, 312 (1990).

29. "Chemisorption of Atomic Hydrogen on Lithium Clusters in the FCC (100), (110), and (111) Symmetries," (with A. S. Hira), Bulletin of the American Physical Society, **35**, 312 (1990).
30. "*Ab Initio* Studies of Neutral K_nNa , Cationic K_nNa^+ , K_nMg , and K_nMg^+ Clusters," (with S. P. Berry and S. D. Altekar), Bulletin of the American Physical Society, **35**, 312 (1990).
31. "An MBPT Study of the Interaction of an O Atom with Lithium Clusters," (with A. S. Hira), Bulletin of the American Physical Society, **35**, 313 (1990).
32. "A Correlation Study of Carbon Clusters," (with M. S. Islam), Bulletin of the American Physical Society, **36**, 353 (1991).
33. "Geometries and Energies of Small Aluminum Clusters in FCC Symmetry," (with B. K. Rao), Bulletin of the American Physical Society, **36**, 506 (1991).
34. "An *Ab Initio* Study of Neutral and Cationic Potassium Clusters," (with K. M. Kanal and I. A. Howard), Bulletin of the American Physical Society, **36**, 653 (1991).
35. "An *Ab Initio* Study of Oxygen Chemisorption on Lithium Clusters," (with A. S. Hira), Bulletin of the American Physical Society, **36**, 854 (1991).
36. "Adsorption of Hydrogen onto Icosohedral Boron Clusters," (with I. A. Howard), Bulletin of the American Physical Society, **36**, 941 (1991).

37. "An *Ab Initio* Study of Alkali Metal Atom Chemisorption on Silicon Clusters," (with S. N. Ekpenuma), Bulletin of the American Physical Society, **36**, 1004 (1991).
38. "A Hartree-Fock Study of Small Carbon Cluster Anions," (with B. K. Rao), Poster Presentation, International Symposium on the Physics and Chemistry of Finite Systems: From Clusters to Crystals, Virginia Commonwealth University, Richmond, Virginia (1991).
39. "Structure and Binding in Small Neutral and Cationic Boron Clusters," (with I. A. Howard and K. M. Kanal), Bulletin of the American Physical Society, **37**, 530 (1992).
40. "A Hartree-Fock Study of Small Carbon Cluster Anions," (with B. K. Rao), Bulletin of the American Physical Society, **37**, 531 (1992).
41. "2-Dimensional Electron Transport Using Discrete Ordinates," (with R. P. Datta and A. S. Hira), Bulletin of the American Physical Society, **37**, 554 (1992).
42. "Sodium Atom Chemisorption on Silicon Surface," (with S. N. Ekpenuma), Poster Presentation, 1992 March Meeting of the American Physical Society.
43. "Structure and Binding in Small Anionic Boron Clusters," (with I. A. Howard), Bulletin of the American Physical Society, **38**, 68 (1993).
44. "Stabilities of Clusters in Two Dimensions," (with B. K. Rao and P. Jena), Bulletin of the American Physical Society, **38**, 69 (1993).

45. "Chemisorption Study of the Interaction of Li and Na Atoms with Si (100) Clusters," (with P. C. Lin and A. S. Hira), Bulletin of the American Physical Society, **38**, 1682 (1993).

46. "An *Ab Initio* Study of Na Chemisorption on the Si (111) Surface," (with M. Mahapatra and A. S. Hira), Bulletin of the American Physical Society, **38**, 1681 (1993).

47. "Spectroscopy of the Li_4^- Cluster," (with B. K. Rao and P. Jena), Bulletin of the American Physical Society, **39**, 415 (1994).

48. "A Correlation Study of Sodium Atom Chemisorption on GaAs (110) Surface," (with K. M. Song and D. C. Khan), Bulletin of the American Physical Society, **39**, 84 (1994).

49. "On the Electronic Structures of GaAs Clusters," (with P. K. Khowash and K. M. Song), Bulletin of the American Physical Society, **39**, 84 (1994).

50. "On the Choice of Basis Sets for the Chemisorption of Hydrogen on Aluminum," (with P. C. Lin, J. Niu and B. K. Rao), International Symposium on the Science and Technology of Atomically Engineered Materials, Virginia Commonwealth University , Richmond , Virginia , 1995.

51. "An *Ab Initio* Study of Alkali Induced Metallization of GaAs (110) Surface," *Invited Lecture*, Fall Meeting of the Texas Section of the American Physical Society, 1996.

52. "A Simulated Annealing Study of Aluminum Clusters," (with C. Gonzales), Bulletin of the American Physical Society, **42**, 462 (1997).

53. "An *Ab Initio* Cluster Study of the Ga Rich GaAs (100) Surface," (with R. Schailey), Bulletin of the American Physical Society, **42**, 785 (1997).
54. "A Density Functional Study of Small Neutral and Cationic Vanadium Clusters," (with X. Wu), Poster Session, 1999 March Meeting of the American Physical Society.
55. "A Study of the Stability and Characterization of Plutonium Dioxide," (with J. C. Boettger), Poster Session, 23rd Annual Actinide Separations Conference, Pasco , Washington , 1999.
56. "An Electronic Structure Study of Solid Plutonium Dioxide," (with J. C. Boettger), Researchers' Conference, Amarillo National Research Center , Amarillo , Texas , 1999.
57. "A Molecular Orbital Study of Plutonium Oxide and Dioxide," (with E. F. Archibong), Researchers' Conference, Amarillo National Research Center , Amarillo , Texas , 1999.
58. "A Hybrid Density Functional Cluster Study of the Bulk and Surface Electronic Structures of Plutonium Monoxide." (with X. Wu), Bulletin of the American Physical Society, **45**, 897 (2000).
59. "An *Ab Initio* Cluster Study of Chemisorption of Atomic Cesium on Ga-Rich GaAs(100) (2x1), (2x2) and β (4x2) Surfaces," (with R. Schailey), Bulletin of the American Physical Society, **45**, 898 (2000).
60. "A Cluster Approach to Hydrogen Chemisorption on the GaAs(100) Surface," (with R. Schailey), Bulletin of the American Physical Society, **45**. 898 (2000).

61. "An Electronic Structure Study of Solid Uranium and Plutonium Dioxides," (with J. C. Boettger), Bulletin of the American Physical Society, **45**, 900 (2000).
62. "An *Ab Initio* Study of Pu – Related Molecular Complexes," (with E. F. Archibong), Bulletin of the American Physical Society, **45**, 960 (2000).
63. "A Density Functional Study of Square and Hexagonal Plutonium Monolayers," (with J. C. Boettger), Bulletin of the American Physical Society, **45**, 1007 (2000).
64. "Density Functional Study of Plutonium Dioxide,"(with X. Wu), Bulletin of the American Physical Society, **46**,766 (2001).
65. "A Hybrid Density Functional Cluster Study of the Bulk and Surface Electronic Structures of PuO₂," (with X. Wu), Bulletin of the American Physical Society, **46**, 486 (2001).
66. "Density Functional Calculations on Hydroxylated Actinide-Oxide Surfaces," (with J. C. Boettger), Sanibel Symposium (2002).
67. "An Electronic Structure Study of the (110) Surface of δ - Pu," (with M. Leonard), Bulletin of the American Physical Society, **47**, 368 (2002).
68. "A Correlation Study of Small Silver Clusters," (with M. N. Huda), Bulletin of the American Physical Society, **47**, 1249 (2002).
69. "*Ab Initio* Modeling of the Endohedral and Exohedral C₆₀ Na₂⁺ Complexes," (with A. S. Hira), Bulletin of the American Physical Society **47**, 1196 (2002).

70. "Anisotropy of Quantum Size Effects in Aluminum (100), (110), (111) Surfaces", (with M.N.Huda), Bulletin of the American Physical Society, **48**, 1029 (2003).
71. "Quantum Size Effects in Thorium (100) and (111) Surfaces " (with M. N .Huda), Bulletin of the American Physical Society, **48**, 1029 (2003).
72. "An *Ab Initio* Study of Alkali-C₆₀ Complexes," (with N. E. Frick and A. S. Hira), Bulletin of the American Physical Society **48**, 106 (2003).
73. "Electronic Structures and Magic Numbers of Small Silver Clusters: A Many Body Perturbation Theoretic Study" (with M. N. Huda), Bulletin of the American Physical Society **48**, 324 (2003).
74. "An *Ab Initio* Cluster Study of Chemisorption of Atomic Oxygen on Ga-Rich GaAs (100) (2x1) and β (4x2) Surfaces," (with M. L. Mayo), Bulletin of the American Physical Society **48**, 489 (2003).
75. "Quantum Size Effects in Hexagonal Plutonium Layers," (with J. C. Boettger), Poster Presentation, Pu2003 Conference, Albuquerque , New Mexico , 2003.
76. "Carbon Dimer in Silicon Cage: A Class of Highly Stable Silicon Carbide Clusters," (with M. N. Huda), Bulletin of the American Physical Society, **49**, 381 (2004).
77. "Novel Silicon-Carbon Fullerene Like Cages: A Class of sp^2 - sp^3 Covalent-Ionic Hybridized Nanosystems," (with M. N. Huda), Bulletin of the American Physical Society, **49**, 384 (2004).

78. "Electronic and Bonding Properties of Hydrogen and Oxygen Adsorption on Uranium Layers," (with M. N. Huda), Bulletin of the American Physical Society, **49**, 949 (2004).
79. "Adsorption of Atomic Hydrogen and Oxygen on δ - Pu Layers," (with M. N. Huda), Bulletin of the American Physical Society, **49**, 950 (2004).
80. "An *Ab Initio* Study of Aluminum Chemisorption on Ga-Rich GaAs (100) (2x1) and β (4x2) Surfaces," (with M. L. Mayo), Bulletin of the American Physical Society **49**, 1095 (2004).
81. "Structure and Bonding in Mixed Silicon-Carbon Nanoclusters: A LDA-DFT Study," (with P. Pradhan), Bulletin of the American Physical Society **49**, 1135 (2004).
82. "An *Ab Initio* Study of H₂ Interaction with the Pu (100) Surface," (with M. N. Huda), Bulletin of the American Physical Society **50**, 378 (2005).
83. "An LAPW Study of δ - Plutonium and the (001) Surface," (with X. Wu), Bulletin of the American Physical Society, **50**, 472 (2005).
84. "A First-Principles Electronic Structure Study of Quantum Size Effects in (111) Films of FCC Plutonium," (with J. C. Boettger), Bulletin of the American Physical Society, **50**, 472 (2005).
85. "An *Ab Initio* Study of Molecular Oxygen Adsorption on Pu (111) Surface," (with M. N. Huda), Bulletin of the American Physical Society, **50**, 472 (2005).

86. "In – Rich Reconstructions of the InSb (100) Surface and Chemisorption of Lithium on the c (8x2) Surface – An *Ab Initio* Study," (with L. G. Sridevi), Bulletin of the American Physical Society, **50**, 140 (2005).
87. "Novel Silicon-Carbon Nanostructures – Electronic Structure Study on the Stability of Si₆₀C_{2n} Clusters," (with A. Srinivasan and M. N. Huda), Bulletin of the American Physical Society, **50**, 302 (2005).
88. "Electronic Structure Studies of Silicon-Carbon Cationic Nanoclusters," (with P. Pradhan), Bulletin of the American Physical Society, **50**, 1169 (2005).
89. "A Density Functional Study of Molecular Oxygen Adsorption and Reaction Barrier on Pu (100) Surface," (with M. N. Huda), Bulletin of the American Physical Society, **50**, 1271 (2005).
90. "Hydrogen Molecule Adsorption and Dissociation on Pu (111) Surface," (with M. N. Huda), Bulletin of the American Physical Society, **50**, 1257 (2005).
91. "An *Ab Initio* Study of the Use of Ag₂⁻ for Catalytic Oxidation of CO," (with P. Dholabhai), Bulletin of the American Physical Society, **50**, 1444 (2005).
92. "An *Ab Initio* Study of Silicon and Germanium Nanotubes," (with P. Pradhan), Bulletin of the American Physical Society, **50**, 1288 (2005).
93. "Fully Relativistic LCGTO-FF Calculations of Quantum Size Effects in Plutonium Films," (with J. C. Boettger), paper presented at the Sanibel, 2005 Meeting.
94. "A Fully-Relativistic Density Functional Study of the Role of 5f Electrons in Chemical Bonding in Transuranium Elements," *Invited Oral Presentation* at

the Contractors' Meeting of the Separations and Heavy Element Chemistry Programs, Division of Chemical Sciences, Geosciences, and Biosciences, United States Department of Energy, Rockville, Maryland (2005).

95. "Novel Silicon-Carbon Nanostructures – An *Ab Initio* Study on the Stability of $\text{Si}_{60}\text{C}_{20}$ Clusters," (with A. Srinivasan and M. N. Huda), Poster Session, Fall 2005 Meeting of the Materials Research Society, Boston , MA .
96. "5f Delocalization of Bulk FCC Americium and the (111) Surface: FP-LAPW Electronic Structure Calculations," (with D. Gao), Oral Presentation, Fall 2005 Meeting of the Materials Research Society, Boston , MA .
97. "A First-Principles Study of the (111), (001), and (110) Surfaces of Delta-Pu," (with H. Gong), Oral Presentation, Fall 2005 Meeting of the Materials Research Society, Boston , MA .
98. "An *Ab Initio* Study of Atomic Oxygen Adsorption on the (100) Surface of Gamma-Uranium," (with P. Dholabhai), Poster Session, Fall 2005 Meeting of the Materials Research Society, Boston , MA .
99. "A Density Functional Study of the Americium (001) Surface," (with D. Gao), Bulletin of the American Physical Society, **51**, 480 (2006).
100. "A Density Functional Study of Carbon Monoxide Adsorption on the (100) Surface of γ – Uranium," (with P. Dholabhai), Bulletin of the American Physical Society, **51**, 480 (2006).
101. "A Density Functional Study of Atomic Oxygen and Carbon Adsorptions on the (100) Surface of γ – Uranium," (with P. Dholabhai), Bulletin of the American Physical Society, **51**, 480 (2006).

102. "Quantum Size Effects in δ – Pu (111) and (110) Films," (with H. R. Gong), Bulletin of the American Physical Society, **51**, 168 (2006).

103. "Novel Silicon-Carbon Nanostructures: A DFT Study on the Stability of $\text{Si}_{60}\text{C}_{2n}$ ($n=3, 10, 12$) Cluster," (with A. Srinivasan and M. N. Huda), Bulletin of the American Physical Society, **51**, 116 (2006).

104. "Silicon-Carbon Nanostructures to Nanotubes," (with M. N. Huda and L. Kleinman), Bulletin of the American Physical Society, **51**, 928 (2006).

105. "The Ground State and Localization of 5f Electrons in α – Pu," (with H. R. Gong), Poster Presentation, Pu Futures – The Science, July 9-13, 2006, Pacific Grove , California .

106. "A First-Principles Electronic Structure Study of the High-Symmetry Surfaces of FCC Americium," (with D. Gao), *Invited Talk*, Pu Futures – The Science, July 9-13, 2006, Pacific Grove , California .

107. "A Density Functional Study of Carbon Monoxide Adsorption on the (100) Surface of Gamma-Uranium," (with P. Dholabhai), Poster Presentation, Pu Futures – The Science, July 9-13, 2006, Pacific Grove , California .

108. "A Comparative *Ab Initio* Electronic Structure Study of FCC δ – Pu and Am II Surfaces," *Invited* Poster Presentation, Third United States Department of Energy – Russian Academy of Sciences Workshop on Basic Actinide Chemistry, July 13-15, 2006, Monterey , California .

109. "A Hybrid Density Functional Study of Armchair SiC Nanotubes," (with K. Alam), Paper Presented at the Fall, 2006 Joint Meeting of the Texas Section of the American Physical Society, October 5-7, 2006, Arlington , Texas .

110. "Relaxation of Actinide Surfaces: An All Electron Study," (with R. Atta-Fynn and P. Dholabhai), Paper Presented at the Fall, 2006 Joint Meeting of the Texas Section of the American Physical Society, October 5-7, 2006, Arlington , Texas .

111. "An *Ab Initio* Full Potential Fully Relativistic Study of Atomic Carbon, Nitrogen, and Oxygen Chemisorption on the (111) Surface of δ - Pu," (with R. Atta-Fynn), Paper Presented at the Fall, 2006 Joint Meeting of the Texas Section of the American Physical Society, October 5-7, 2006, Arlington, Texas.

112. "A FP-LAPW Study of Atomic Carbon, Nitrogen, and Oxygen Chemisorption on the (100) Surface of δ - Pu," (with R. Atta-Fynn), Paper Presented at the Fall, 2006 Joint Meeting of the Texas Section of the American Physical Society, October 5-7, 2006, Arlington , Texas .

113. "A Hybrid Density Functional Study of Si Nanotubes," (with S. Rathi), paper presented at the March, 2007 Meeting of the American Physical Society.

114. "A Hybrid Density Functional Study of SiC Nanotubes," (with K. Alam), paper presented at the March, 2007 Meeting of the American Physical Society.

115. "A FP-LAPW Study of Atomic Chemisorption on the (111) Surface of δ - Pu," (with R. Atta-Fynn), paper presented at the March, 2007 Meeting of the American Physical Society.

116. "A FP-LAPW Study of Atomic Chemisorption on the (100) Surface of δ - Pu," (with R. Atta-Fynn), paper presented at the March, 2007 Meeting of the American Physical Society.

117. "An *Ab Initio* Full Potential Fully Relativistic Study of the (0001) Surface of Double Hexagonal Close Packed Americium," (with D. Gao), paper presented at the March, 2007 Meeting of the American Physical Society.
118. "A Fully-Relativistic Density Functional Study of the Role of 5f Electrons in Chemical Bonding in Transuranium Elements," *Invited* Poster Presentation at the Contractors' Meeting of the Separations and Heavy Element Chemistry Programs, Division of Chemical Sciences, Geosciences, and Biosciences, United States Department of Energy, Annapolis, Maryland (2007).
119. "A Fully-Relativistic Density Functional Study of the Role of 5f Electrons in Chemical Bonding in Transuranium Elements," *Invited Speaker*, Contractors' Meeting of the Condensed Phase and Interfacial Molecular Sciences Programs, Division of Chemical Sciences, Geosciences, and Biosciences, United States Department of Energy, Warrenton, Virginia (2007).
120. "A Hybrid Density Functional Study of Zigzag SiC Nanotubes." (with K. Alam), poster presented at the March, 2008 Meeting of the American Physical Society, <http://meetings.aps.org/Meeting/Mar08>, p. 262.
121. "A Density Functional Study of Atomic Hydrogen and Oxygen Chemisorptions on the (0001) Surface of Double Hexagonal Close Packed Americium," (with P. Dholabhai and R. Atta-Fynn), paper presented at the March, 2008 Meeting of the American Physical Society, <http://meetings.aps.org/Meeting/Mar08>, p. 435.
122. "Adsorption and Dissociation of Molecular Oxygen on the (0001) Surface of Double Hexagonal Close Packed Americium," (with P. Dholabhai and R. Atta-Fynn), poster presented at the March, 2008 Meeting of the American Physical Society, <http://meetings.aps.org/Meeting/Mar08>, p. 142.

123. "On the Electronic Structures of Ge-Based Nanotubes," (with S. Rathi), poster presented at the March, 2008 Meeting of the American Physical Society, <http://meetings.aps.org/Meeting/Mar08>, p. 136.
124. "Atomic Adsorptions on the (020) Surface of α - Pu: A Density Functional Study," (with R. Atta-Fynn), poster presented at the March, 2008 Meeting of the American Physical Society, <http://meetings.aps.org/Meeting/Mar08>, p. 144.
125. "Relaxation of the (111) Surface of δ -Pu and Effects on Atomic Adsorption: An *Ab Initio* Study," (with R. Atta-Fynn), paper presented at the March, 2008 Meeting of the American Physical Society, <http://meetings.aps.org/Meeting/Mar08>, p. 196.
126. "On the Electronic and Geometric Structures of Armchair GeC Nanotubes: A Hybrid Density Functional Study," (with S. Rathi). paper presented at the March, 2008 Meeting of the American Physical Society, <http://meetings.aps.org/Meeting/Mar08>, p. 358.
127. "An *Ab Initio* Study of the Interaction of Transition Metal Atoms with Single-Wall Armchair SiC Nanotubes," (with K. Alam), paper presented at the March, 2008 Meeting of the American Physical Society, <http://meetings.aps.org/Meeting/Mar08>, p. 514.
128. "Evolution of SiC Nano-Cluster from Carbon Fullerene: A Density Functional Theory Study." (with M. N. Huda), poster presented at the March, 2008 Meeting of the American Physical Society, <http://meetings.aps.org/Meeting/Mar08>.
129. "A Hybrid Density Functional Study of Pure Ge and GeC Nanotubes: Zigzag Configuration," (with S. Rathi), poster presented at the March, 2009 Meeting of the American Physical Society, <http://meetings.aps.org/Meeting/MAR09>, p144.

130. "Adsorption and Dissociation of Water on the (0001) Surface of DHCP Americium," (with P. Dholabhai), poster presented at the March, 2009 Meeting of the American Physical Society, <http://meetings.aps.org/Meeting/MAR09>, p. 277.
131. "Hydrogen Adsorption on the (020) Surface of alpha-Pu : A Computational Study," (with M. Islam), poster presented at the March, 2009 Meeting of the American Physical Society, <http://meetings.aps.org/Meeting/MAR09>, p 277
132. "A First Principles Study of the Adsorption and Dissociation of CO₂ on the delta-Pu (111) Surface," (with R. Atta-Fynn), poster presented at the March, 2009 Meeting of the American Physical Society, <http://meetings.aps.org/Meeting/MAR09>, p 278.
133. "A Hybrid Density Functional Study of delta-Pu," (with R. Atta-Fynn), paper presented at the March, 2009 Meeting of the American Physical Society, <http://meetings.aps.org/Meeting/MAR09>, p 313
134. "An LDA+U Study of the Photoemission Spectra of the Ground State Phases of Americium and Curium," (with M. Islam), paper presented at the March, 2009 Meeting of the American Physical Society, <http://meetings.aps.org/Meeting/MAR09>, p 278.
135. "Does Water Adsorb Molecularly or Dissociatively on a Plutonium Surface," (with R. Atta-Fynn), paper presented at the March, 2009 Meeting of the American Physical Society, <http://meetings.aps.org/Meeting/MAR09>, p 364.
136. "On the Interplay between Spin Polarization, Orbital Polarization, and Spin-Orbit Coupling in Actinides from Pa to Cm," (with M. Islam), poster presented at the March, 2009 Meeting of the American Physical Society, <http://meetings.aps.org/Meeting/MAR09>, p 399.

- 137.** “Adsorption and Dissociation of Molecular Hydrogen on the (0001) Surface of DHCP Americium,” (with P. Dholabhai), paper presented at the March, 2009 Meeting of the American Physical Society, <http://meetings.aps.org/Meeting/MAR09>, p 417.
- 138.** “Can Silicon Carbide Nanotubes be Effective Medium for Hydrogen Storage,” (with S. Mukherjee), paper presented at the March, 2009 Meeting of the American Physical Society, <http://meetings.aps.org/Meeting/MAR09>, p 505.
- 139.** “A Fully-Relativistic Density Functional Study of the Role of 5f Electrons in Chemical Bonding in Transuranium Elements,” *Invited Oral Presentation* at the Contractors’ Meeting of the Separations and Heavy Element Chemistry Programs, Division of Chemical Sciences, Geosciences, and Biosciences, United States Department of Energy, Warrenton, Virginia (2009).
- 140.** “Electronic, Structural, and Thermodynamic Properties of Mixed Actinide Dioxides (U, Pu, Am) O₂ from Hybrid Density Functional Theory,” (with L. Ma), poster presented at the March, 2010 Meeting of the American Physical Society, <http://meetings.aps.org/Meeting/MAR10>, Bulletin of the American Physical Society, **55**, p 161.
- 141.** “A Hybrid DFT Description of the Ground State Properties of Americium I,” (with R. Atta-Fynn), poster presented at the March, 2010 Meeting of the American Physical Society, <http://meetings.aps.org/Meeting/MAR10>, Bulletin of the American Physical Society, **55**, p 161.
- 142.** “A Hybrid Density Functional Study of Double-Walled Armchair SiC Nanotubes,” (with K. Adhikari), paper presented at the March, 2010 Meeting of the American Physical Society, <http://meetings.aps.org/Meeting/MAR10>, Bulletin of the American Physical Society, **55**, p 350.

143. "Electronic, Structural, and Thermodynamic Properties of Actinide Dioxides, "(with L. Ma and R. Atta-Fynn), paper presented at the March, 2010 Meeting of the American Physical Society, <http://meetings.aps.org/Meeting/MAR10>, Bulletin of the American Physical Society, **55**, p 443
144. "Quantum Size Effects in the Properties of Non-Magnetic Americium-I (0001) Surface: A Hybrid DFT Study, " (with R. Atta-Fynn), paper presented at the March, 2010 Meeting of the American Physical Society, <http://meetings.aps.org/Meeting/MAR10>, Bulletin of the American Physical Society, **55**, p 580.
145. "Ab Initio Studies of Atomic and Molecular Adsorptions on Plutonium Surfaces," Plenary Speaker, Pu Futures 2010 Conference, Keystone, Colorado, 20-23 September, 2010. Abstract published in p. 212-213, American Nuclear Society, ISBN 978-0-89448-082-9.
146. "Magnetic and Thermodynamic Properties of Americium II: An Ab Initio Study," (with J. Wang and Li Ma), poster presented at the March, 2011 Meeting of the American Physical Society, www.aps.org/meetings/march, Bulletin of the American Physical Society, **56**, p. 163.
147. "An Ab Initio Study of Rare Gases in Uranium Dioxide," (with Li Ma), poster presented at the March, 2011 Meeting of the American Physical Society, www.aps.org/meetings/march, Bulletin of the American Physical Society, **56**, p. 169
148. "An Ab Initio Study of Bulk γ - U and the (100) Surface," (with D. Morrison), paper presented at the March, 2011 Meeting of the American Physical Society, www.aps.org/meetings/march, Bulletin of the American Physical Society, **56**, p. 251.
149. "A Hybrid Density Functional Study of Capped Silicon Carbide Nanotubes," (with K. Adhikari), paper presented at the March, 2011 Meeting of the

American Physical Society, www.aps.org//meetings/march, Bulletin of the American Physical Society, **56**, p. 269.

- 150.** “Adsorption and Dissociation of Molecular Oxygen on α – Pu (020) Surface: A Density Functional Study,” (with J. Wang), paper presented at the March, 2011 Meeting of the American Physical Society, www.aps.org//meetings/march, Bulletin of the American Physical Society, **56**, p. 381.
- 151.** “A First-Principles Study of SiGe Nanotubes,” (with P. Wanaguru), poster presented at the March, 2011 Meeting of the American Physical Society, www.aps.org//meetings/march, Bulletin of the American Physical Society, **56**, p. 419.
- 152.** “An *Ab Initio* Study of SiC Double-Walled Nanotubes of Types 2 and 3,” (with K. Adhikari), poster presented at the March, 2011 Meeting of the American Physical Society, www.aps.org//meetings/march, Bulletin of the American Physical Society, **56**, p. 420.
- 153.** “An *Ab Initio* Study of Atomic Hydrogen and Oxygen Adsorptions on Armchair Si Nanotubes,” (with H. Chen), poster presented at the March, 2011 Meeting of the American Physical Society, www.aps.org//meetings/march, Bulletin of the American Physical Society, **56**, p. 420.
- 154.** “An *Ab Initio* Study of α – Pu,” (with S. Hernandez), paper presented at the March, 2011 Meeting of the American Physical Society, www.aps.org//meetings/march, Bulletin of the American Physical Society, **56**, p 532.
- 155.** “An *Ab Initio* Study of $\text{PuO}_{2\pm 0.25}$, $\text{UO}_{2\pm 0.25}$, $\text{U}_{0.5}\text{Pu}_{0.5}\text{O}_{2\pm 0.25}$,” (with Li Ma), paper presented at the March, 2011 Meeting of the American Physical Society, www.aps.org//meetings/march, Bulletin of the American Physical Society, **56**, p 533.

- 155.** “*Ab Initio* Studies of Si_mGe_n ($m+n \leq 5$) Nanoclusters,” (with S. Duesman), paper presented at the March, 2011 Meeting of the American Physical Society, www.aps.org//meetings/march, Bulletin of the American Physical Society, **56**, p 573.
- 156.** “A Nanocluster Based Study of Silicon Carbide Nanocones,” (with K. Adhikari), paper presented at the March, 2012 Meeting of the American Physical Society, www.aps.org//meetings/march, Bulletin of the American Physical Society, **57**, p 459.
- 157.** “Anomalous Dependence of Band Gaps of Binary Nanotubes on Diameters,” (with K. Adhikari and M. N. Huda). poster presented at the March, 2012 Meeting of the American Physical Society, www.aps.org//meetings/march, Bulletin of the American Physical Society, **57**, p 503.
- 158.** “Molecular Hydrogen and Oxygen Interactions with Si Nanotubes,” (with H. Chen), paper presented at the March, 2012 Meeting of the American Physical Society, www.aps.org//meetings/march, Bulletin of the American Physical Society, **57**, p 658.
- 159.** “Structural Properties and Stability of Double-Walled Armchair Silicon Nanotubes,” (with H. Chen), poster presented at the March, 2012 Meeting of the American Physical Society, www.aps.org//meetings/march, Bulletin of the American Physical Society, **57**, p 573.
- 160.** “A First Principles Study of Water Adsorption on alpha – Pu (020) Surface,” (with J. Wang), paper presented at the March, 2012 Meeting of the American Physical Society, www.aps.org//meetings/march, Bulletin of the American Physical Society, **57**, p 146.

- 161.** “First Principles Study of Adsorption and Dissociation of CO₂ on alpha-Pu (020) Surface, (with J. Wang), poster presented at the March, 2012 Meeting of the American Physical Society, www.aps.org//meetings/march, Bulletin of the American Physical Society, **57**, p 512.
- 162.** “Four Types of Single-Walled SiGe Nanotubes: Existence and Stability,” (with P. Wanaguru), poster presented at the March, 2012 Meeting of the American Physical Society, www.aps.org//meetings/march, Bulletin of the American Physical Society, **57**, p 513.
- 163.** “A DFT Study of Atomic Hydrogen and Oxygen Chemisorption on gamma-U Surface,” (with D. Morrison), paper presented at the March, 2012 Meeting of the American Physical Society, www.aps.org//meetings/march, Bulletin of the American Physical Society, **57**, p 638.
- 164.** “Performance of Hybrid Density Functional Theory for Alpha- versus Delta-Pu, “ (with S. Hernandez), poster presented at the March, 2012 Meeting of the American Physical Society, www.aps.org//meetings/march, Bulletin of the American Physical Society, **57**, p 518.

Seminars and Invited Presentations:

Brooklyn College of the City University of New York

Condensed Phase and Interfacial Molecular Sciences Meeting, Department of Energy

Department of Energy Laboratory, Idaho Falls

Indian Association for the Cultivation of Science, Calcutta , India

Mathematics Department, University of Texas at Arlington

Michigan Technological University

Naval Research Laboratory, Washington , D. C.

Physics Department, University of Texas at Arlington

Princeton University

Saha Institute of Nuclear Physics, Calcutta , India

Tarleton State University

Technical University of Vienna , Austria

Texas Tech University

Books Authored

“Probing 5f Electrons: A Relativistic DFT Study of Americium Surfaces,” (with P. Dholabhai), Lambert Academic Publishing, Germany, 2009.

Books Edited

“*Nanoclusters and Nanostructured Surfaces,*” (Ed. Asok K. Ray, American Scientific Publishers, 2010).

Editorial Service

Associate Editor, *Journal of Nanoscience and Nanotechnology*, American Scientific Publishers.

Associate Editor, *Journal of Computational and Theoretical Nanoscience*, American Scientific Publishers.

Guest Editor. *Silicon Carbide Nanostructures : Theory and Computation*, *Journal of Computational and Theoretical Nanoscience*, American Scientific Publishers.

Member of the Editorial Board, *Transport Theory and Statistical Physics*, Taylor and Francis Publishing.

Member of the Editorial Advisory Board, *Recent Patents on Materials Science*, Bentham Science Publishers.

Member of the Editorial Board, *Journal of Nano Energy and Power Research*, American Scientific Publishers.

Referee Service:

Canadian Journal of Physics

Chemical Physics Letters

Computational and Theoretical Chemistry

Department of Defense Review Panel

Department of Energy

European Physical Journal B

Heteroatom Chemistry

IEEE – Transactions on Electron Devices

International Journal of Quantum Chemistry

Israel Science Foundation

Journal of Alloys and Compounds

Journal of Applied Physics

Journal of Nanoscience and Nanotechnology

Journal of Computational Chemistry

Journal of Computational and Theoretical Nanoscience

Journal of Molecular Structure: Theochem

Journal of Nuclear Materials

Journal of Photochemistry and Photobiology

Journal of Physics A

Journal of Physics B

Journal of Physical Chemistry

Journal of Physics: Condensed Matter

Journal of Physics and Chemistry of Solids

Journal of the Electrochemical Society

National Science Foundation

National Science Foundation Review Panel

Optics Communications

Petroleum Research Foundation

Physica B

Physica E

Physical Review B

Physical Review Letters

Physics Letters A

Proceedings of the International Symposium on the Physics and Chemistry of
Small Clusters, Richmond , Virginia

Proceedings of the Materials Research Society

Solid State Sciences

Structural Chemistry

Surface Science

Session Chair, Non-Metallic Clusters, March 1992 Meeting of the American Physical Society

Session Chair, Fall 2006 Joint Meeting of the Texas Section of the American Physical Society

Texas Journal of Science

Theoretical Chemistry Accounts

Transport Theory and Statistical Physics

United States Department of Energy, Innovative and Novel Computational Impact on Theory and Experiment (INCITE) Scientific Review Panel, 2007.

United States Civilian Research and Development Foundation

Grants and Related Activities

“Safety Analysis for Pipeline Transmission of Hydrogen,” Los Alamos Scientific Laboratory, \$5,000.00 (1978-79).

Shell Faculty Grant , Michigan Technological University, \$250.00 (1981-82).

“Total Energy of Solids and the Generator Coordinate Method”, Michigan Technological University Summer Faculty Grant, \$2,500.00 (1982).

“Properties of Three-Dimensional Energetic Solids and Molecular Crystals ,” (with A. B. Kunz, D. R. Beck, R. S. Weidman and T. O. Woodruff), Office of Naval Research, \$60,000.00 (1981-82).

“Computation of Electron and Photon Transport in Layered Media by Invariant Imbedding,” (with P. Nelson), Air Force Office of Scientific Research, \$36,000.00 (1983-84).

“Theoretical Studies of Solids Under Extreme Conditions,” (with J. L. Fry, P. C. Pattnaik and G. L. Fletcher), Air Force Office of Scientific Research, \$247,000.00 (1983-85).

“Transport Properties of $(\text{Bi,Sb})_2(\text{Te,Se})_3$,” (with J. L. Fry and G. L. Fletcher), Marlow Industries, \$30,000.00 (1984).

Organized Research Fund, The University of Texas at Arlington , \$2,000.00 (1984).

Summer Faculty Grant, Organized Research Fund, The University of Texas at Arlington , \$5,000.00 (1985).

Research Travel Grant, The University of Texas at Arlington , \$1,000.00 (1986).

Cray Research Corporation Colloquium Grant (with A. H. Weiss), \$2,000.00 (1986-87).

“Analysis of Eruption Clouds Detected by Satellites,” (with S. Self), National Science Foundation, \$78,000.00 (1987-88).

“Molecules to Clusters to Solids – An *Ab Initio* Study,” The Welch Foundation, \$247,000.00 (1987-96).

Research Travel Grant, The University of Texas at Arlington , \$500.00 (1987).

Research Travel Fellowship, University of East Anglia , Norwich , United Kingdom , \$2,000.00 (1987).

Research Travel Grant, The University of Texas at Arlington , \$500.00 (1988).

Research Initiation Grant for 20 CPU hours, The John von Neumann National Supercomputer Center (1988).

“An Analysis of Cluster Physics,” Research Support Grant, 500 CPU Hours on an IBM 3090 and \$5,000.00 Travel Expenses, IBM Los Angeles Scientific Center (1988).

Cray Research Corporation Colloquium Grant (with A. H. Weiss), \$5,000.00 (1987-89).

“Computational Techniques for Microscopic Models of Transport in Semiconductors”, Cray Research, \$66,000.00 (1989-90).

Research Travel Grant, The University of Texas at Arlington , \$1,500.00 (1990).

“A New Approach to Transport Theoretic Analysis of Radiation Damage in Microelectronic Structures,” (with P. Nelson), Texas Advanced Technology Program, \$121,819.00 (1990-91).

Guest Professorship, The Technical University of Vienna , Austria , \$5,000.00 (1990).

Visiting Research Fellowship, Oxford University , England , \$2,000.00 (1991).

“A Computational Database for Scattering Cross-Sections in Semiconductors,” 325 CPU Hours on a Cray YMP 8/64, Cray Research (1992).

“A Parallel Transport Algorithm for the Cray YMP,” 75 CPU hours on a Cray YMP 8/64, Cray Research (1992).

"Molecules to Clusters to Solids- An *Ab Initio* Study," National Science Foundation, Pittsburgh Supercomputing Center, 600 CPU Hours on a Cray C90 (1994).

"A Theoretical Study of Alkali Atom Interactions with Silicon Surfaces," Cray Research, \$7,500.00 Direct Funds and \$30,000.00 in Computer Time (1995).

"A Density Functional Study of Alkali Interactions with the GaAs (110) Surface," 300 CPU Hours on a Cray C90, National Science Foundation Pittsburgh Supercomputing Center (1995).

"Parallel Electron Transport Softwares on a Cray T3D, 10,000 Units on a Cray T3D, National Science Foundation Pittsburgh Supercomputing Center (1995).

"Acquisition of Quantum: A High Performance SGI Workstation," (with J. L. Fry and I. A. Howard), \$50,000.00, Office of Computing and Information Technology, The University of Texas at Arlington (1995).

"An *Ab Initio* Study of Chemisorption on Metal and Semiconductor Surfaces," 5000 units on a SGI Power Challenge and 1000 units on a HP Convex Exemplar, National Center for Supercomputing Applications, Urbana, Illinois (1996).

"Acquisition of Personal Computers," \$30,000.00, Office of Computing and Information Technology, University of Texas at Arlington (1996).

"Numerical Discretization Schemes for the Fokker-Planck Equation," Los Alamos National Laboratory, Department of Energy, \$24,576.00 (1997).

Visiting Research Fellowships, Princeton University , Princeton , New Jersey , \$12,000.00 (1998-99).

“Modeling of Solid State and Thermodynamic Properties of Actinides,” (with J. M. Sanchez), \$151,864.00, Amarillo National Research Center , Department of Energy (1999).

“A Density Functional Study of the Surface Electronic Behavior of Actinide Metals,” \$680,000.00 (2001-2012), Welch Foundation, Houston, Texas.

“A Fully Relativistic Density Functional Study of the Role of 5f Electrons in Chemical Bonding in Transuranium Elements,” \$694,000.00 (2003-2010), United States Department of Energy.

Sub-contracts pending with Los Alamos National Laboratory and Air Force Research Laboratory.

Proposals Written (Not Funded)

“Theoretical Studies of Energetic Materials,” (with D. S. Marynick and J. L. Fry).

“Novel Theoretical Approaches to the Studies of Conducting Polymers.” (with D. S. Marynick and J. L. Fry).

“Studies of Conducting Polymers”.

“Modeling of Ultra Small Semiconductor Devices,” (with P. Nelson, C. W. Myles and H. D. Victory).

“Physics of Sub-Micron Semiconductor Devices and Hot Electron Transport,”
(with C. W. Myles).

“*Ab Initio* Studies of Metal Clusters”.

“Integration of Code Systems AMBER, CHARM and GAMESS”.

“Positron Studies of Defects in Compound Semiconductors,” (with R. N. West
and J. H. Kaiser).

“A New Approach to the Study of Chemisorption on Metal Surfaces”.

“A Computational Database for Scattering Cross-Sections in Semiconductors”.

“A Parallel Transport Algorithm for the Cray YMP”.

“Design of New Materials from Studies of Interactions of Heteroatoms with
Conventional and Novel Semiconductors,” (with I. A. Howard).

“Parallel Programming in Electron Transport: Experiments in SIMD and MIMD
Architectures”.

“Damage Prevention, Detection, and Growth Retardation in Smart Laminated
Composites,” (with S. P. Joshi and W. S. Chan).

“Impurities in Borides and Small Boron Clusters,” (with I. A. Howard).

“An *Ab Initio* Study of Induced Metallization at Semiconductor Surfaces”.

“Serial and Parallel Programming for Electron Transport in Multi-Dimensions”.

“An *Ab Initio* Study of Atomic and Molecular Chemisorption on Aluminum Surfaces”.

“Transition Metal Clusters: A Parallel Monte Carlo Simulated Annealing Study”.

“Acquisition of Advanced Computer Systems for Visualization of Complex Physical Phenomena,” (with T. Black, R. Magnusson, T. Maldonado and Q. Zhang).

“An *Ab Initio* Study of Metal Oxides and Molecular Adsorption”

“A Novel Approach to Electron and Photon Transport in Biological Tissues,” (with R. Glickman, R. Horomoto and D. Sardar).

“First-Principles Investigations on the Deposition and Growth of Novel Dielectric Thin-Film Materials,” (with Q. Zhang).

“Novel Parallel Algorithms for Nuclear Well Logging: The PANTHER Consortium,” (with P. Nelson and N. Abdurrahman).

“Acquisition of Advanced Computing Facilities for Investigations of Complex Condensed Phase Systems,” (with I. A. Howard and Q. Zhang).

“Novel Techniques for the Simulation of Particle Transport on Modern Parallel Computational Platforms,” (with P. Nelson, S. Oliviera and N. Abdurrahman).

“Development of Parallel Algorithms for Three-Dimensional Transport Codes,” (with S. Oliviera and N. Abdurrahman).

“Coupled Electron-Photon Transport in Multi-Dimensions: A Parallel Discrete Ordinates Study”.

“A Novel Cluster Study of Oxide Surfaces and Molecular Adsorption”.

“Novel CBN- and AlSiP- Based Materials,” (with D. J. Klein).

“Boron Diffusion in Silicon-Based Novel Dielectric Materials,” (with Q. Zhang).

“First-Principles Investigation of Novel Dielectric Materials,” (with Q. Zhang).

“Towards A Systematic Understanding of the Electronic Structures of the Actinide Molecular Complexes”

“Development of Tools for Nanoparticle Based Technologies”

“Quasi-Continuum Modeling Limits for Nanoscale Systems”

“Mechanisms of Nanoscale Breakdowns in the Vicinity of a Macroscopically Defined Interface Crack,” (with S. P. Joshi)

“Structure Property Relations in Nanostructured Alumina-Titania Composites,” (with S. P. Joshi)

“ Physics Analysis Frontier Center ,” (with A. White, K. De, and A. Brandt)

“A Novel Algorithm for Direct 4-Component Relativistic Self-Consistent-Field (SCF) Method : Applications to Condensed Matter”

“Acquisitions of Advanced Computing Facilities for Investigations of Complex Condensed Phase Systems”

“Simulations in Electronic Structures for Silicon-Carbide sp^2 - sp^3 Hybridized Nanosystems”

“A Novel Class of Carbon Embedded Silicon Nanostructures”

“Integrative Graduate Education and Research in Super- and Parallel-Computing in Particles and Fluids,” (with Q. Zhang, Y. Su, C. Liu, H. Shan, J. Zhu, and J. Horwitz).

“Beyond Carbon Nanotubes: A Hybrid Density Functional Electronic Structure Study,” (with L. Burggraf)

“Towards the Next Generation of Scintillators: An *Ab Initio* Study”

“An *Ab Initio* Full Potential Fully Relativistic Electronic Structure Study of Actinide Nitrides as Nuclear Fuels”

“Beyond Standard Density Functional Theory: Hybrid Density Functional Theory and LDA+U Methods for Applications to Actinides and Actinide Compounds”

“Towards a Complete understanding of the Thermodynamic Properties of UO₂, PuO₂, and MOX Advanced Actinide Fuels based on *Ab Initio* Quantum Mechanical Studies”

Post-Doctoral Fellows Directed

Dr. E. Archibong

Dr. R. Atta-Fynn

Dr. A. Bakshai

Dr. R. P. Datta

Dr. S. N. Ekpenuma

Dr. D. Gao

Dr. H. R. Gong

Dr. A. S. Hira

Dr. S. R. Kafle

Dr. D. C. Khan

Dr. Li Ma

Dr. M. Mahapatra

Dr. J. Wang

Dr. X. Wu

Graduate Students Directed

Thesis/Dissertation Titles

Mr. T. Cathey (M. S. 1987)

“Numerical Evaluation of Feynman Propagators in Imaginary Time”

Mr. A. S. Hira (M. S. 1987)

“Cluster Modeling of Hydrogen Interaction with Lithium Surfaces”

Ms. L. Glaze (M. S. 1988)

“A Diffusion Model Applied to Remote Sensing Studies of Volcanic Eruption Plumes”

(Co-Advisor: Dr. S.

Self, Department of

Geology, The University

of Texas at Arlington)

Ms. S. Berry (M. S. 1989)

“Mass Spectra and Leptonic Decay Widths of the CC and BB Systems”

Ms. S. Altekar (M. S. 1989)

“An *Ab Initio* Study of Potassium and Mixed Potassium/Magnesium Clusters”

Mr. M. Islam (D. Sc. 1989)

“An *Ab Initio* Study of Carbon and Germanium Clusters”

Mr. A. S. Hira (Ph. D. 1990)

“Many Body Perturbation Theory Applied to Hydrogen Interaction with Lithium Surfaces”

Ms. J. Tripathi (M. S. 1990)

“A Class of Quark Confinement Potentials”

Ms. K. Kanai (M. S. 1991)

“On the Existence and Stability of Potassium Clusters”

- Mr. T. Kellogg (M. S. 1993) "One Dimensional Electron Transport: Application to Electron Backscattering"
- Mr. P. Lin (M. S. 1993) "Stabilities of Adsorption Sites and Charge Transfers at the Li/Si (100) and Na/Si (100) Surfaces"
- Mr. R. P. Datta (Ph. D. 1993) "Coupled Electron Photon Transport: A Multi-Dimensional Discrete Ordinates Study"
- Mr. K. M. Song (Ph. D. 1994) "An *Ab Initio* Study of Alkali Metal Adsorption on Gallium Arsenide (110) Surface"
- Ms. S. D. Altekar (Ph. D. 1995) "Parallel Programming in Electron Transport: A Cray YMP Study"
- Ms. M. Panda (M. S. 1997) "Interactions of Alkali Atom with GaAs (110) Surface: A Density Functional Approach"
- Mr. R. Schailey (Ph. D. 1999) "An *Ab Initio* Cluster Study of Chemisorption of Atomic Cesium and Hydrogen on Reconstructed Surfaces of Gallium Rich Gallium Arsenide (100)"
- Ms. X. Wu (Ph. D. 2001) "Density Functional Theory Applied to d- and f- Electron Systems"

<u>Mr. N. E. Frick</u> (M. S. 2002)	“An <i>Ab Initio</i> Study of Alkali-C ₆₀ Complexes”
<u>Mr. M. N. Huda</u> (M.S. 2002)	“A Perturbation-Theoretic and Coupled-Cluster Study of Silver Nanostructures”
<u>Mr. M. L. Mayo</u> (M. S. 2003)	“A Many Body Perturbation Theoretic Study of Atomic Oxygen and Aluminum Chemisorption on GaAs (100) (2x1) and β (4x2) Surfaces”
<u>Mr. M. N. Huda</u> (Ph. D. 2004)	“A Relativistic Density Functional Study of the Role of 5f Electrons in Atomic and Molecular Adsorptions on Actinide Surfaces”
<u>Ms. P. Pradhan</u> (M. S. 2005)	“Nanoclusters to Nanotubes: An <i>Ab Initio</i> Study”
<u>Ms. L. G. Sridevi</u> (M. S. 2005)	“On a Class of ABCS”
<u>Mr. P. Dholabhai</u> (M. S. 2005)	“On the Behavior of 5f Electrons”
<u>Mr. A. Srinivasan</u> (M. S. 2005)	“On the Existence and Stability of Carbon-Based Silicon Fullerenes: A Density Functional Theoretic Study”

- Mr. K. M. Alam (M. S. 2008) “Silicon Carbide Nanotubes: Promises Beyond Carbon Nanotubes”
- Mr. S. Rathi (M. S. 2008) “Germanium Based Nanotubes: Fact or Fiction?”
- Mr. P. Dholabhai (Ph. D. 2008) “Probing the *5f* Electrons: A Relativistic DFT Study of Americium Surfaces”
- Mr. S. Mukherjee (M. S. 2008) “Can Silicon Carbide Nanotubes Be Effective Medium for Hydrogen Storage?”
- Ms. S. Duesman (M. S. 2011) “On the Electronic and Geometric Structure Properties of Silicon Germanium Nanocluster: A Hybrid Density Functional Theoretic Study”

Current Undergraduate Students

Ms. D. Baker

Ms. W. Hall

Ms. M. Lee

Current Graduate Students:

Mr. K. Adhikari

Mr. H. Chen

Ms. S. Hernandez

Ms. D. Morrison

Mr. P. Wannaguru

Current Post-Doctoral Fellows

Dr. J. Wang

Graduate Thesis/Dissertation Committees:

J. Alleto (M. S.)

O. Aniltruk (Ph. D.)

S. Ayyalasomayajula (M. S.)

H. Che (M. S.)

C. Ethridge (D. Sc.)

N. Guler (M. S.)

N. Hozhabri (D. Sc.)

C. Hyer (Ph. D.)

C. Jiang (M. S.)

M. Jibaly (D. Sc.)

K. Lee (M. S.; D. Sc.)

E. Livesay (Ph. D.)

R. Mittal (M. S.; Ph. D.)

M. Morse (M.S.)

S. Mukherjee (Ph. D.)

K. O'Brien (Ph. D.)

R. Ramsey (Ph. D.)

J. Rejczek (Ph. D.)

R. Sharma (M. S.)

S. Shin (M. S.)

M. Sosbee (Ph. D.)

H. Tu (M. S.)

X. Wang (M. S.)

D. Wu (M. S.; Ph. D)

Y. Xia (M. S.)

A. Zhao(Ph. D.)

Undergraduate Students Directed:

S. Anderson

M. Averitte

K. Balasubramanium

D. Baker

S. Bell

M. Eberwine

C. Erhorn

A. Flores

E. Gonzales

C. Harenza

A. Hendrix

K. Honza

E. James

N. Kohli

R. Minyard

A. Naqvi

L. Page

P. Pappas

A. Passi

R. Pathak

D. Price

J. Richards

D. Wagner

K. Wright

Courses Taught:

Texas Tech University
Semesters

Mathematics 137,138

Title

Mathematical Analysis
for Business Majors

3

Physics 141, 142

General Physics I and II

7

University of Florida

Title

Quarters

Physics 2050

General Physics I

4

Physics 2052

General Physics II

2

Physics 2053

Applied Physics II

1

Michigan Tech. University

Title

Quarters

Physics 204	Physics for Engineers I	2
Physics 209	General Physics III	2
<u>University of Texas at Arlington</u>	<u>Title</u>	<u>Semesters</u>
Physics 1441	General College Physics I	20
Physics 1442	General College Physics II	2
Physics 1445	Introductory Astronomy I	1
Physics 3313	Modern Physics	4
Physics 4117	Individual Learning by Seminar	1
Physics 4181	Special Problems	6
Physics 4281	Special Problems	5
Physics 4326	Introduction to	1

Quantum Mechanics

Physics 5190	Physics Colloquium	4
Physics 5307	Quantum Mechanics I	11
Physics 5308	Quantum Mechanics II	7
Physics 5310	Statistical Mechanics	1
Physics 5311	Mathematical Methods in Physics I	7
Physics 5312	Mathematical Methods in Physics II	5
Physics 5316	Solid State Physics II	1
Physics 5319	Mathematical Methods in Physics III	6
Physics 5393	Readings in Physics	4

Physics 5394	Research	32
Physics 5694	Research	22
Physics 5698	Thesis	20
Physics 6999	Dissertation	9
Physics 6302	Methods of Applied Physics II: Computers in Physics	1

Technical University Title Semesters
Of Vienna

Chemistry	Density Functional Theory	1
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Honors and Organizations:

Government of India National Scholar (1967).

Who's Who in Frontiers of Science and Technology (1990).

Member of the American Physical Society (1978 – cont.).

Member of American Nuclear Society (1984-87).

Member of the Materials Research Society (2005-cont.)

Member of Sigma Pi Sigma (1973-77).

Member of the Society for Industrial Applications of Mathematics (1977-1979).

Consultant, RELTEC Corporation, Dallas , Texas (1997).

Who's Who in America, 2005-2012.

College of Science Research Excellence Award, University of Texas at
Arlington, 2004 -2010.

Who's Who in Science and Engineering, 2006-2011

Nominated for Distinguished Long-Term Research Award, University of Texas
at Arlington, 2005, 2006, 2007.

Distinguished Record of Research or Creativity Award, University of Texas at

Arlington, 2011.

Who's Who in the World, 2007.

Phi Kappa Phi "Recognized Professor", 2011

Committees, Physics Department, The University of Texas at Arlington :

Member of Undergraduate Studies Committee (1978-79).

Member of the Committee on Text of Modern Physics (1984-85).

Member of the Committee on Industrial Relations (1985-86).

Chair or Co-Chair of the Committee on Computer Use (1984-2002).

Member of the Committee on Faculty Search (1984-96, 2000- 2006, 2008-2009).

Member of the Committee on Undergraduate Curriculum (1985-87; 1989-90).

Member of the Graduate Studies Committee (1985-cont.).

Co-Chair of the Colloquium Committee (1986-89, 2000-01).

Co-Chair of the Graduate Recruitment Committee (1987-92).

Member of the Teaching Committee (1988-91).

Chair of the Graduate Studies Committee (1991-98).

Member of the Library Committee (1985-96, 1999-cont.).

Member of the Research Committee (1985-96, 1999-2004).

Chair of the Research Committee (2004-2006).

Chair of the Graduate Admissions Committee (1988-98, 1999-2004, 2008-2010).

Member of the Graduate Admissions Committee (2004-cont.).

Doctoral Graduate Advisor (1988-92, 2001- 2003).

Graduate Advisor (2008-2012)

Member of the Tenure and Promotion Committee (1988-96; 2000-02; 2003-2010).

Chair of the Tenure and Promotion Committee (1996-97; 2000-01).

Chair, Graduate Studies Subcommittee (1991-95).

Member of the Awards Committee (1999-2001, 2008-cont.).

Member of the Long Range Planning Committee (1999-2001).

Member of the Accommodation Committee (1997-2002).

Chairman's Committee (1997-1998; 1999-2001; 2004-cont.).

M. S. Graduate Advisor (1999-2001).

Chair, Theory Search Committee (2004).

Member of Strategic Planning Committee (2003-cont.).

Member of the Astronomy Instructor Search Committee (2004-2005).

Member of the Task Force on Computer Security (2005-2006).

Chair of the Associate Chair Review Committee (2004-2005).

Chair of the Chair Review Committee (2008-2009).

Chair of the Committee for the Acquisition of a Beowulf Parallel Cluster (2005).

Member of the Computer Cluster Committee (2006-2008)

Member of the Periodic Review of Tenure Committee (2006-2008)

Member of the Periodic Review of Tenure Appeals Committee (2000-cont.)

Member of the Science Hall Renovation/Reprogramming (2005-2009)

Member of the Tenure and Promotion Guidelines Committee (2006-2009).

University Committees:

Associate Member of the Graduate Faculty (1984-88).

Member of the Graduate Faculty (1988-cont.).

Member of the Undergraduate Curriculum Committee, College of Science (1989-90).

Member of the Center for High-Performance Committee User Advisory Committee, The University of Texas System (1989-94).

Member of the Ad Hoc Supercomputing Facilities Committee (1988-94; 1996-cont.).

Member of the Registration, Scheduling and Calendar Committee (1998-2000).

Member of the College of Science Tenure and Promotion Committee (2000-2002; 2004-2006, 2009-2010).

Member of College of Science Research Committee (2005-2007).

Member of the University Graduate Assistants' Task Force (2005-cont.).

Faculty Mentoring Program (2004-2005).

Chair, High Performance Computing Users Group (2008 – cont.).

UTA Representative to the Texas Advanced Computing Center User
Advisory

Group (2008 – cont.)

Co-Chair of the Research Advisory Committee, 2011.

UTA Representative to the Faculty Outreach Working Group, University of
Texas Research Cyberinfrastructure Project (2011-cont.)