Mahdi Sanati June 2024

Department of Physics & Astronomy, Lubbock, TX 79423-1051
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Education

Ph.D, Physics, University of Cincinnati, OH, USA (1999)
Thesis: "*A theoretical study of the omega-phase transformation in metals*"
Advisor: Professor Frank Pinski
Co-Advisors: Robert C. Albers and Avadh Saxena (Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM)

Research Experiences and Employments

- Associate Professor, Department of Physics & Astronomy, Texas Tech University, Lubbock, TX (2010-present)
- Guest Scientist, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM (2007-present)
- Assistant Professor, Department of Physics & Astronomy, Texas Tech University, Lubbock, TX (2004-2010)
- Postdoctoral Researcher, Department of Physics & Astronomy, Texas Tech University, Lubbock, TX, (2002-2004)
- Postdoctoral Researcher, National Renewable Energy Laboratory, Golden, CO (2000-2002)
- Postdoctoral Researcher, Department of Applied Mathematics, University of Western Ontario, London, Canada (1999-2000)
- Graduate Research Assistant, Los Alamos National Laboratory, NM (1996-1999)

Teaching Awards

- Professor of Year Award, Society of Physics Students, Department of Physics & Astronomy, TTU, Lubbock, TX (2010)
- Professor of Year Award, Society of Physics Students, Department of Physics & Astronomy, TTU, Lubbock, TX (2023)

Teaching Experiences, and Courses

Texas Tech University (2004-present)

1) Advanced Electromagnetic Theory (Graduate)
2) Advanced Quantum Mechanics (Graduate)
3) Analytical Mechanics (Graduate)
4) Applied Quantum Mechanics (Graduate)
5) Computational Physics (Graduate)
6) Electromagnetic Theory (Graduate)
7) Group Theory in Physics (Graduate)
8) Methods in Physics (Graduate)
9) Modern Electricity and Magnetism (Graduate)
10) Quantum Mechanics II (Graduate)
11) Partial Differential Equations of Mathematical Physics (Graduate)

12) Problem Solving in Physics (Graduate)
13) Statistical Mechanics (Graduate)
14) Electricity and Magnetism I (undergraduate)
15) Electricity and Magnetism II (undergraduate)
16) General Physics I (Undergraduate)
17) General Physics II (Undergraduate)
18) Mathematical Methods in Physical Science I (Undergraduate)
19) Principles of Physics I (Undergraduate)
20) Principles of Physics II (Undergraduate)
21) Principles of Physics III (undergraduate)
22) Principles of Physics IV (undergraduate)
23) Solar System Astronomy (Undergraduate)
24) Statistical and Thermal Physics (Undergraduate)
25) Stellar Astronomy (Undergraduate)

University of Western Ontario, ON, Canada (1999-2000)

1) Materials Modeling (Graduate)
2) Linear Algebra for Engineers (Undergraduate)

Research Mentoring

Postdoc

West, Damien (2008)

Chair of Doctoral Committees

1) Karkash, Ahmed A. A. (2024) Molecular Dynamics Studies of Metallic Bulks, Surfaces, and Nanostructures
2) Diaz, Leopoldo III (2022) A first-principles study of transition metal surfaces
3) Alsalmi, Omar (2019) First-Principles Study of the Binary Ti-Al Phase Diagram at High Temperature

Chair of Masters Committees

1) Aslan, Ali N. (2023) Computational Secondary Electron Emission Analysis of Ag and Au under Oxygen-Carbon Surface Contamination
2) Alsharari, Sami (2023) Theoretical Studies of Cu (110) Surface with the Different Carbon Coverages
3) Vincent III, Timothy Mark (2021) Cu and Ag in Si: the elusive Cu0 and *Cu0 defects
4) Brown, Madeline (2021) Secondary Electron Emission of Clean and Hydrogen Layered Nickel Surfaces
5) Mulherin, Olivia (2017) Theoretical Study of the Elastic and Thermal Properties of the AuCd Shape Memory Alloy
6) Alsalmi, Omar (2014) Phase stability of XZn (X = Cu, Ag, and Au) B2 phase alloys

Undergraduate Capstone Projects:

1) Musella, Anthony (2024)

2) Auer, Garrett (2021)
3) Viljoen, Pieter (2020)
4) Wagner, Madeleine (2020)
5) Alvarez, Steven (2019)
6) Puac, Jeniffer (2019)
7) Hirsch, Rachel (2013)

Publications (Refereed Journals)

1) L. Diaz, A. Krakash, S. Alshahri, R. P. Joshi, E. Schamiloglu, M. Sanati, *Importance of the Surface Morphology on the Secondary Electron Emission: A Case Study of Cu covered with Carbon, Carbon Pairs, or Graphite,* Sci. Rep. 13 (Nature Publishing Group), 8260 (2023). https://doi.org/10.1038/s41598-023-34721-8
2) M. Maille, N. C. Dennis, Y. M. Pokhrel, M. Sanati, and R. P. Joshi, *Simulation Studies of Secondary Electron Yield with Electron Transport from Cu (110) Surfaces Containing C_2, N_2, CO_2, or NO_2 Adsorbates,* Front. in Mater. Vol. 10 (2023) | https://doi.org/10.3389/fmats.2023.1145425
3) L. Diaz, R. C. Albers, A. Saxena, and M. Sanati, *Dipolar effects on the work function of an alkali-iodide overlayer (XI, X= Li, Na, K, Rb, and Cs) on tungsten surfaces,* Phys. Scrip. 27 (9), 093511 (2023) doi 10.1088/1402-4896/acba54
4) M. Brown, L. Diaz, A. Aslan, M. Sanati, S. Portillo, E. Schamiloglu, R. P. Joshi, *Carbon-oxygen surface formation enhances secondary electron yield in Cu, Ag and Au*, Sci. Rep. (Nature Publishing Group), 15808 (2022) https://doi.org/10.1038/ s41598-022-19924-9
5) M. Brown, M. Sanati, R.P. Joshi, *Combined first-principles-Monte Carlo analysis to evaluate the effect of surface hydrogen on the secondary electron yield of nickel*, J. Appl. Phys. 131 (10), 103301 (2022) doi: 10.1063/5.0080721
6) D. Guo, S. N. Sami, L. Diaz, M. Sanati, R. P. Joshi, *Evaluation of electron currents from cesium-coated tungsten emitter arrays with inclusion of space charge effects, workfunction changes, and screening* J. Vac. Sci. & Tech. B, 39 (5) 054201 (2021) https://doi.org/10.1116/6.0001185
7) W. Milestone, D. Guo, M. Sanati, K. M. Dowling, S. Hau-Riege, L. F. Voss, A. M. Conway, R. P. Joshi, *Monte Carlo transport analysis to assess intensity dependent response of a carbon-doped GaN photoconductor* J. Appl. Phys. 129 (19), 195703 (2021) https://doi.org/10.1063/5.0040173
8) S. N. Sami, M. Sanati, and R. P. Joshi, *Simulations of hydrogen outgassing and sticking coefficients at a copper electrode surface: Dependencies on temperature, incident angle and energy,* Phys. Rev. Res. 3, 013203 (2021) doi: 10.1103/ PhysRev Research.3.013203
9) X. Qiu, L. Diaz, M. Sanati, J. Mankowski, J. Dickens, A. Neuber, and R. P. Joshi *Coupled analysis to probe the effect of angular assignments on the secondary electron yield (SEY) from copper electrodes,* Phys. Plas. 27 (9), 093511 (2020) https://doi.org /10.1063/5.0010389
10) S. N. Sami, L. Diaz, M. Sanati, and R. P. Joshi, *Simulations of field emission from copper electrodes with inclusion of oxygen surface layer and work function changes based on first-principles calculations,* J. Appl. Phys. 128:223302 (2020) https://doi.org/10.1063/5.0031568

11) H. K. A. Nguyen, M. Sanati, and Ravi Joshi, *Probing changes in secondary electron yield from copper electrodes due to surface defects and changes in crystal orientation,* J. Appl. Phys. 126:123301 (2019) https://doi.org/10.1063/1.5113642
12) O. Alsalmi, M. Sanati, R.C. Albers, T. Lookman, and A. Saxena, *First-Principles Study of Phase Stability of bcc XZn (X=Cu, Ag, and Au) Alloys,* Phys. Rev. M. 2, 11 (2018) doi: 10.1103/PhysRevMaterials.2.113601
13) M. Sanati, R.C. Albers, T. Lookman, and A. Saxena, *First-order versus second-order phase transformation in AuZn,* Phys. Rev. B., 88, 024110 (2013) doi: 10.1103/ Phys RevB.88.024110
14) M. Sanati, R.C. Albers, T. Lookman, and A. Saxena, *Elastic constants, phonon density of states, and thermal properties of UO_2,* Phys. Rev. B., 20, 465206 (2011) doi: 10.1103/PhysRevB.84.014116
15) M. Sanati, R.C. Albers, T. Lookman, and A. Saxena, *First-principles study of stability of the bcc and ω phases of a low Al concentration $Nb_{1-x}Al_x$ alloy*, J. Phys. Condensed Matter., 23, 295501 (2011) doi: 10.1088/0953-8984/23/29/295501
16) M. Sanati, D. West, and R.C. Albers, *Calculations of displacive ω-phase transformations in Ti-Al alloys with Nb additions at finite temperature*, J. Phys. Condensed Matter, 20, 465206 (2008) doi:10.1088/0953-8984/20/46/465206
17) N. Gonzalez Szwacki, M. Sanati, S.K. Estreicher, *Two FeH pairs in n-type Si and their implications: A theoretical study*, Phys. Rev. B, 78, 113202 (2008) https://doi.org/10.1103/PhysRevB.78.113202
18) S.K. Estreicher, M. Sanati, and N. Gonzalez Szwacki, *Iron in silicon: interaction with radation defects, carbon, and oxygen*, Phys. Rev. B, 77, 125214 (2008) https://doi.org/10.1103/PhysRevB.77.125214
19) K. Biswas, C.W. Myles, M. Sanati, and G.S. Nolas, *Thermodynamics of gust free Si_{136} and Ge_{136} Clathrates: first-principles study*, J. Appl. Phys., 104, 033535 (2008) doi: 10.1063/1.2960580
20) S.K. Estreicher, M. Sanati, and N. Gonzalez Szwacki, *Fundamental Interaction of Fe in silicon: First-Principles Theory*, Sol. St. Phen. XII, 131-133, 233 (2008) https://doi.org/10.4028/www.scientific.net/SSP.131-133.233
21) M. Sanati, D. West, and R.C. Albers, *Electronic structure, chemical ordering, and phase stability of the ω-phase in a Ti_3Al_2X (X=Nb, V) alloy*, Phys. Rev. B 76, 174101 (2007) doi: 10.1103/PhysRevB.76.174101
22) M. Sanati, D. West, and R.C. Albers, *First-principles study of ω-phase formation in the Ti_3Al_2V system*, J. Phys. Condensed Matter 19, 386221 (2007) stacks.iop.org/JPhysCM/19/386221
23) M. Sanati and A. Zunger, *Evolution of $L1_2$ ordered domains in fcc Cu_3Au Alloy*, J. Phys. Condensed Matter 19, 086201 (2007) http://iopscience.iop.org/0953-8984 /19/8/086201
24) M. Sanati, N. Gonzalez Szwacki, and S. K. Estreicher, *Interstitial Fe in Si and its interactions with hydrogen and shallow dopants*, Phys. Rev. B 76, 125204 (2007) https://doi.org/10.1103/PhysRevB.76.125204
25) M. Sanati and S.K. Estreicher: *First-principles study of iron and iron pairs in Si*, Phys. B 401-402, 105 (2007)

26) A. Carvalho, R. Jones, M. Sanati, S. K. Estreicher, J. Coutinho, and P. R. Briddon, *First-principles investigation of a bistable boron-oxygen interstitial pair in Si*, Phys. Rev. B 73, 245210 (2006) https://doi.org/10.1103/PhysRevB.73.245210
27) S.M. Myers, A.F. Wright, M. Sanati, and S.K. Estreicher: *Theoretical properties of the N vacancy in p-type GaN(Mg,H) at elevated temperatures*, J. Appl. Phys. 99, 11 (2006) https://doi.org/10.1063/1.2195894
28) M. Sanati and S.K. Estreicher: *Oxygen-Boron Complexes in Si*, Phys. B 376-377, 133 (2006) https://doi.org/10.1016/j.physb.2005.12.035
29) S.K. Estreicher and M. Sanati: *Predicting the energetics of Defects at T>0K*, Phys. B 376-377, 940 (2006) https://doi.org/10.1016/j.physb.2005.12.234
30) R.N. Pereira, B. Bech Nielsen, M. Stavola, M. Sanati, S.K. Estreicher, and M. Mizuta: *Local Vibrational Modes of Hydrogen in GaN: Observation and Theory*, Phys. B 376-377, 464 (2006) https://doi.org/10.1016/j.physb.2005.12.119
31) A.F. Wright, S.M. Myers, M. Sanati, and S.K. Estreicher: *Formation of V_NH and MgV_NH in p-type GaN(Mg,H)*, Phys. B 376-377, 477 (2006) https://doi.org/10.1016/j.physb.2005.12.122
32) S.K. Estreicher and M. Sanati: *D, H, and Muin GaN, Theoretical Predictions at finite temperature*, Phys. B 374, 363 (2006) https://doi.org/10.1016/j.physb.2005.11.102
33) G. Davies, S. Hayama, S. Hao, B. Bech Nielsen, J. Coutinho, M. Sanati, S.K. Estreicher, and K.M. Itoh: *Host isotope effects mid-infra-red optical transitions in silicon*, Phys. Rev. B 71, 115212/1-7 (2005)
34) G. Davies, S. Hayama, S. Hao, J. Coutinho, S.K. Estreicher, M. Sanati and K.M. Itoh: *Lattice isotope effects on the widths of optical transition in silicon*, J. Phys. Condensed Matter, 17, S2211-S2217 (2005) doi: 10.1088/0953-8984/17/22/008
35) R.K. Kremer, M. Cardona, E. Schmitt, J. Blumm, S.K. Estreicher, M. Sanati, M. Bockowski, A. Grzegory, T. Suski, and A. Jezowski: *Heat capacity of α- GaN: Isotope effects*, Phys. Rev. B 72, 075209/1-6 (2005) https://doi.org/10.1103/PhysRevB.72.075209
36) S.K. Estreicher, D. West, and M. Sanati: *Identification of $*Cu_0$ as a metastable configuration of the $\{Cu_s,Cu_i\}$ pair in Si*, Phys. Rev. B 72 (Rapid Communication), R121201/1-4 (2005) https://doi.org/10.1103/PhysRevB.72.121201
37) M. Sanati and S.K. Estreicher: *Temperature and sample dependence of the binding free energies of complexes in crystals: the case of acceptor-oxygen complexes in Si*, Phys. Rev. B 72, 165206/1-8 (2005) https://doi.org/10.1103/PhysRevB.72.165206
38) M. Cardona, R.K. Kremer, M. Sanati, S.K. Estreicher, and T.R. Anthony: *Measurement of the heat capacity of diamond with different isotopic Compositions*, Sol. St. Comm. 133, 465-468 (2005) https://doi.org/10.1016/j.ssc.2004.11.047
39) S.K.Estreicher, M. Sanati, D. West, and F. Ruymgaart: *Thermodynamics of impurities in semiconductors*, Phys. Rev. B 70, 125209/1-10 (2004) https://doi.org/10.1103/PhysRevB.70.125209
40) M. Sanati and S.K. Estreicher: *Specific heat and entropy of GaN*, J. Phys. Condensed Matter 16, L327-L331 (2004) doi: 10.1088/0953-8984/16/28/L02
41) M. Sanati, S.K. Estreicher, and M. Cardona: *Isotopic-dependence of the heat capacity of c-C, Si, and: An ab-initio calculation* Sol. St. Comm. 131, 229-233 (2004) https://doi.org/10.1016/j.ssc.2004.04.043

42) S.K. Estreicher and M. Sanati: *Calculating the properties of defects at finite temperatures*, in: Defects and Diffusion in Semiconductors-An Annual Retrospective VII, ed. D.J. Fisher, Defects and Diffusion Forum 230-232, 47 (2004) https://doi.org /10.4028/ www.scientific.net/DDF.230-232.47
43) M. Sanati and S. K. Estreicher: *Defects in silicon: the role of vibrational entropy*, Sol. St. Comm. 128/5, 181 (2003) https://doi.org/10.1016/j.ssc.2003.08.005
44) M. Sanati and S. K. Estreicher: *First-principles thermodynamic of defects in Silicon*, Phys. B 340-342, 630 (2003) https://doi.org/10.1016/j.physb.2003.09.158
45) M. Sanati, G. Hart, and A. Zunger: *Ordering Tendencies in Octahedral MgO-ZnO Alloys*, Phys. Rev. B 68, 155210 (2003) https://doi.org/10.1103/PhysRevB.68.155210
46) M. Sanati and A. Saxena: *Landau theory of domain walls for one dimensional asymmetric potentials*, Am. J. Phys., 71, 1005 (2003) https://doi.org/ 10.1119/ 1.1578064
47) M. Sanati, L. G. Wang, and A. Zunger: *Adaptive Crystal Structures*, Phys. Rev. Lett., 90, 045502-1 (2003) https://doi.org/10.1103/PhysRevLett.90.045502
48) Zunger, L. G. Wang, G. Hart, M. Sanati: *Obtaining Ising-like Expansion for Binary Alloys from First-Principles*, Mod. Sim. Mat. Sci. Eng. 10, 685 (2002) doi: 10.1088/0965-0393/10/6/306
49) M. Sanati, A. Saxena, and T. Lookman : *Domain wall modeling of bcc to hcp reconstructive phase transformation in early transition metals*, Phys. Rev. B, 64, 092101 (2001) https://doi.org/10.1103/PhysRevB.63.224114 (80% contribution)
50) M. Sanati, A. Saxena, T. Lookman, and R. C. Albers: *Landau free energy for bcc-hcp reconstructive phase transformation*, Phys. Rev. B, 63, 224114 (2001) https://doi.org/10.1103/PhysRevB.64.092101
51) M. Sanati, R. C. Albers, and F. J. Pinski: *ω-phase formation in NiAl and Ni_2Al alloys*, J. Phy. Condensed Matter 13, 5378 (2001) doi: 10.1088/0953-8984/13/22/328
52) A. Saxena, M. Sanati, , and R. C. Albers: *Domain walls in bcc to hcp Reconstructive phase transformations*, Materials Science and Engineering A, 273-275, 226 (1999) https://doi.org/10.1016/S0921-5093(99)00376-7
53) M. Sanati and A. Saxena: *Half-kink lattice solution of the φ^6 model*, J. Phy. A, 32, 4311 (1999) doi: 10.1088/0305-4470/32/23/309
54) M. Sanati and A. Saxena: *Modeling of domain walls in ferroelectric polymers*, Ferroelectrics, 222, 113 (1999) https://doi.org/10.1080/00150199908014806
55) M. Sanati and A. Saxena: *Domain walls in ω-phase transformation*, Physica D,123, 368 (1998) https://doi.org/10.1016/S0167-2789(98)00135-3
56) M. Sanati, R. C. Albers and F. J. Pinski: *Electronic and crystal structure of NiTi Martensite*, Phys. Rev. B, 58, 13950 (1998) https://doi.org/10.1103/ PhysRevB.58. 13590

Publications (submitted)

1) A. Karkash, L. Diaz, R. C. Albers, A. Saxena, and M. Sanati *Atomistic mechanism for hydrogen outgassing from Al and Cu FCC metal surfaces under thermal treatment: Failure of diffusion-limited and recombination-limited models*, Phys. Rev. B.
2) Y. Pokhrel, Y. Iqbal, S. Chakraborty Shrestha, M. Sanati, and R, Joshi, *Coupled Monte Carlo Density Functional Theory Calculations of Cold and Laser Assisted Electron Field Emission from Graphene Coated Copper Cathode,* J. App. Phys.

Publications (Conferences)

1) M. Sanati and R.C. Albers, *B2 to ω-phase transformations in Ti_3Al_2Mo alloy: a first-principles approach*, ICOMAT 08, MRS publication, (2009)
2) S.K. Estreicher, M. Sanati, and D. Backlund, *Domain Fe (Ni, Ti) in silicon: the visible, the hidden, and the (partially) passivated*, 18th Workshop on c-Si Solar Cells & Modules, ed. B.L. Sopori, NREL, 46 (2008)
3) M. Sanati and S.K. Estreicher: *Fundamental interactions involving Fe in Si,* 16th Workshop c-Si Solar Cell Materials and Processes (Denver, CO 8/06), NREL/BK 520-40424, 30-33 (2007)
4) M. Sanati and S.K. Estreicher: *Theoretical studies of boron-oxygen complexes in silicon,* 14th Workshop c-Si Solar Cell Materials and Processes (Winter Park, CO 8/04), NREL/BK 520-36622, 180 (2004)
5) D. West, M. Sanati, and S.K. Estreicher: *Temperature-dependence of the dissociation energy of copper pairs in Si,* 14th Workshop c-Si Solar Cell Materials & Processes (Winter Park, 8/04), NREL/BK 520-36622, 184-187 (2004)
6) M. Sanati and S.K. Estreicher: *Theory of defects in silicon solar cells at finite temperatures,*13th Workshop c-Si Solar Cell Materials and Processes (Vail, CO 8/03), NREL/BK 520-3443, 106-109 (2003)

Publications (books)

1) S.K. Estreicher and M. Sanati: *Dynamical Matrices and Free Energies*, in Theory of Defects in Semiconductors, ed. D.A. Drabold and S.K. Estreicher (Springer, Berlin, 2007), p. 95-113

Professional Presentations

Invited Talks

1) "*Importance of Surface Morphology on Electron Emission of Materials",* Northern Illinois University, DeKalb, IL (2023)
2) "*Secondary Electron Emission of Clean and Hydrogen Layered Nickel Surfaces",* Angelo State University, San Angelo, TX (2021)
3) "*First-Principles study of Phase Transformation in Materials",* Angelo State University, San Angelo, TX (2020)
4) Keynote: "*Solitons in Condensed Matter Physics: Landau Theory of Domain Walls for One-dimensional Asymmetric Potentials"*, 4th UMT International Conference on Pure and Applied Sciences, Lahore, Pakistan (2018)
5) Keynote: "*First-Principles study of Phase Transformation in AuZn Shape Memory Alloy"*, 2nd UMT International Conference on Pure and Applied Sciences, Lahore, Pakistan (2017)
6) "*Density Functional Theory and its Application in Materials",* Trinity University, San Antonio, TX (2014)
7) "*First-Principles Thermodynamics of AuZn System*", The North American Calorimetry Conference (CALCON), Santa Fe, NM (2009)
8) "*B2 to ω-phase transformations in Ti_3Al_2Mo alloy: a first-principles approach*", International Conference on Martensitic Transformation, Santa Fe, NM (2008)

9) "*First-Principles Thermodynamics of Fe Defect in Silicon*", International Conference on Defects in Semiconductors-24 Albuquerque, NM (2007)
10) "*Density Functional Theory and its Application in Alloys*", Sam Houston University, Houston, TX (2006)
11) Keynote: "*First-Principles Thermodynamics of Defects in Silicon*", International Conference on Defects in Semiconductors-22 Aarhus, Denmark (2003)

Conferences

1) "*First-Principles Studies of Hydrogen Diffusion Mechanisms in FCC Metals: Al and Cu as Case Studies",* APS March Meeting (2024)
2) "*Selecting Incident Electron Pulse Parameters Forsurface Cleaning to Remove Adsorbates",* IEEE International Conference on Plasma Science (ICOPS) (2023)
3) "*Strain Driven Work Function Reduction in the XI/W (X= Li, Na, K, Rb, and Cs) Systems",* APS March Meeting (2023)
4) "*Effect of Cs and CsI on the low-index surfaces of W",* APS March Meeting (2022)
5) "*Effect of electric field on the electron field emission current densities of Cu and Cu-O systems: A First-Principle Approach",* APS March Meeting (2021)
6) "*A first-principles study of the physical properties and secondary electron emission of 4d and 5d FCC metal surfaces with and without a vacancy defect",* APS March Meeting (2020)
7) "*First-Principles Study of Phase Stability of bcc XZn (X = Cu, Ag, and Au) Alloys",* APS March Meeting (2018)
8) "*Magnetic Landau free energy density for the bcc-hcp phase transformation",* APS March Meeting (2015)
9) "*B2 decomposition of X5Al (X= Sc, Ti, V, Cr, Y, Zr, Nb, and Mo) system, A First-Principles Study",* APS March Meeting, Texas Section (2008)
10) "*Structural phase transformations in Ti_3Al_2Nb system, a first-principles approach",* APS March Meeting (2007)
11) "*Fundamental interactions involving Fe in silicon",* 16th Workshop on Crystalline Silicon Solar Cells and Modules: Materials and Processes (2006)
12) "*Structure, electrical activity, and thermal stability of acceptor-oxygen complexes in Si solar cells",* 14th Workshop on Crystalline Silicon Solar Cells and Modules: Materials and Processes (2005)
13) *"Structure, electrical activity, and thermal stability of acceptor-oxygen complexes in Si solar cells"* 14th Workshop on Crystalline Silicon Solar Cells and Modules: Materials and Processes (2004)
14) *"Theoretical study of boron-oxygen complexes in silicon"* 14th Workshop on Crystalline Silicon Solar Cells and Modules: Materials and Processes (2004)
15) "*New Stable Crystal Structures for Cu-Au and Ni-Pt Alloy Systems",* APS Meeting, Texas Section (2003)
16) *"Theory of defects in silicon solar cells at finite temperatures"* 13th Workshop on Crystalline Silicon Solar Cells and Modules: Materials and Processes (2003)
17) "*LDA-Prediction of New Stable Crystal Structures within= 0A= the Cu-Au and Ni-Pt Alloy Systems",* APS March Meeting (2002)
18) "*Phase-Stability and Electronic Structure of MgO-ZnO Alloys",* APS March Meeting (2002)

19) "*Obtaining Mixed-Basis Ising-Like Expansions of Binary Alloys from First Principles",* APS March Meeting (2002)
20) "*Modeling of growth of $L1_2$-ordered domains in fcc Cu_3Au alloy",* APS March Meeting (2001)
21) "*ω-phase Formation in Group III, IV, and V Transition Metals",* APS March Meeting (2000)
22) "*Exact solutions for a class of asymmetric potentials: application in physical sytems",* APS Four Corner Meeting, Albuquerque, NM (1998)
23) "*Displacive and Diffusive Transformations in the Formation of the Ni_2Al",* APS March Meeting (1998)
24) "*ω-Phase Formation in Ni-Al Systems",* APS March Meeting (1998)
25) "*Domain walls in bcc-to-hcp reconstructive phase transformation",* APS March Meeting (1998)
26) "*ω-Phase Formation in TiAl and Ti_3Al_2Nb Alloys",* APS March Meeting (1997)

Conferences and Workshops

- Organizer: "*First International Workshop on Materials Science and Modeling*" Dubai, UAE (2014) Sponsored by INTERMEAST, UAE Airlines, and Texas Tech University
- Session Chair: "*The 5th International Conference on Clean Energy and Electrical Systems"* Tokyo, Japan (2023)

Grants

Funded

- PI (100%): Advanced Research Program of The State of Texas, *Formation of ω-phase in Ti-Al-X (X=Nb, V, Ta, Mo) systems*, $75,000 (2006-2009)
- Co-PI (20%): DOD - Air Force Office of Scientific Research, *Studies of Electrode-Plasma Effects on Breakdown at RF Frequencies*, $348,600 (2019-2022)
- Co-PI (30%): DOD - Office of Naval Research, *New Anode Materials for High Lethality HPM Sources*, $ 273,522 (2022-2025)
- Co-PI (20%): DOD - Air Force Office of Scientific Research, *Electron Emission for Nanoemitter Arrays Using Theory and Molecular Level*, $ 358,061 (2022-2025)

Unfunded

- PI (100%): US Department of Energy, *Modeling physical, mechanical, and thermal properties of nuclear fuels*, $780,791.
- PI (100%): Norman Hackerman Advanced Research Program, *Modeling of thermal properties of nuclear fuels: A First-Principles Approach*, $150,000
- PI (100%): The Welch Foundation, *Effects of hybridization and chemical ordering on phase stability of transition metals aluminides*, $150,000
- PI (100%): Petroleum Research Fund, *Chemical ordering and first-principles thermodynamics of Ti-Al-V system*, $30,000

Travel Grant

Theoretical Division, Los Alamos National Laboratory: $2,500/year (2007-present)

Under Preparation

PI (20%): US Department of Energy, MINORITY SERVING INSTITUTIONS PARTNERSHIP PROGRAM (MSIPP) *Quantum Material Quest: A Consortium for Advanced Materials Manufacturing (QMQ-CAMM)* ($5,000,000.00)

Services

Departmental

1) Graduate Recruiter, Physics Department, TTU (2007-present)
2) Graduate Committee, Physics Department, TTU (2007-present)
3) PhD qualifying exam committee, TTU (2004-present)

Reviewer (journals)

1) Acta Crystallographica
2) Journal of Applied Physics
3) Journal of Metals and Alloys
4) Metals
5) Physica B
6) Physica Scripta
7) Philosophical Magazine
8) Physical Review Journals

Reviewer (books)

1) "**Modern Quantum Mechanics**" by Sakurai and Napolitano (Cambridge University Press)
2) "**College Physics**" by Giordano 2/e (Cengage)

Reviewer (proposals)

1) American Chemical Society Petroleum Research Fund
2) National Science Foundation
3) US Department of Energy (Basic Sciences)