CURRICULUM VITAE

Krishna Muralidharan

Associate Professor

Department of Materials Science and Engineering University of Arizona

CHRONOLOGY OF EDUCATION

Doctorate of Philosophy, Materials Science and Engineering

University of Arizona, August 2004

Minor: Chemistry

Dissertation: Molecular Dynamics Simulations of Brittle Fracture in Amorphous Silica

Master of Science, Materials Science and Engineering

University of Florida, August 2000

Thesis: Molecular Dynamics Studies of Bulk Self-Diffusion in β-SiC

M.Sc., Physics

Indian Institute of Technology- Madras, India, June 1997

Thesis: Magnetic Susceptibility and Electrical Resistivity of Rare Earth-Transition Metal Alloys

B.Sc Physics

University of Madras, Madras, India, June 1995

CHRONOLOGY OF EMPLOYMENT

05/16-present	Associate Professor, Department of Materials Science and Engineering University of Arizona, Tucson, AZ
08/10-05/16	Assistant Professor, Department of Materials Science and Engineering University of Arizona, Tucson, AZ
10/07-08/10	Assistant Research Professor, Department of Materials Science and Engineering University of Arizona, Tucson, AZ
04/06-10/07	Research Associate, Department of Materials Science and Engineering University of Arizona, Tucson, AZ
11/04-04/06	Postdoctoral Associate, Quantum Theory Project University of Florida (UF), Gainesville, Fl
09/04-03/05	Postdoctoral Fellow, Department of Physics (concurrent with appointment at UF) University of New Mexico, Albuquerque, NM
02/03-08/04	Staff Member/Graduate Research Assistant, MST 8, Los Alamos National Labs Los Alamos, NM

SERVICE AND OUTREACH

Local/State Outreach

- Hosted two lectures on energy sustainability to the general public (UA Science Café, Spring 2012) and high-school students (UA Science Café, Fall 2011).
- Interviewed and featured in two articles on renewable energy storage by the Arizona Daily Star (2011).

National/International Outreach

• Featured on PBS, Phoenix regarding compressed air energy storage in Spring 2011.

Departmental Committees

- Student Advisory Committee (Advising Junior students since 2014).
- Serving on the Undergraduate Course Committee (UCC) from 2011. Chair of the UCC since 2015.
- MSE faculty in-charge of the Engineering camp for high school students (2017)

University Committees

- Serving on the University-wide Research Computing Council.
- Faculty search committee for positions in LPL, Chemical and Environmental Engineering, Materials Science and Engineering

Professional Service

- Reviewer for Journal Articles (Journals listed below)
 Philosophical Magazine, Journal of crystal growth, Applied Physics Letters, AIP Advances, J.Acoustical
 Society of America, Journal of Physics, Theoretical Chemistry Accounts, Chemical Physics Letters, J. Noncrystalline solids, Philosophical Transactions, Solid-State Ionics, J.Phys: Condensed Matter, Solid-state
 communications, Modeling and Simulation in MSE, Physica B, Surface Science, Journal of Chemical Physics,
 Computational Materials Science, Applied Physics Letters, Scientific Reports, Physica E, Materials Research
 Express, Materials Corrosion, Materials Science and Engineering B, ACS Nano, Optics Express, Ionics,
 Nanocomposites, J. Physical Chemistry
- Reviewer for NSF-SEES Panel
- Reviewer for NASA-Emerging Worlds
- Reviewer for NSF-DMR-Career
- Reviewer for DOE-Basic Energy Sciences

Conferences/Workshop Organization

- Symposium organizer, Glass and Optical Materials Division, American Ceramic Society (2017)
- Session chair, Glass and Optical Materials Division, American Ceramic Society (2017)
- Session chair Pacrim, American Ceramic Society (2017).
- Lead organizer for the 2-day workshop on Integrated Computational Materials Science and Engineering."
 Jointly hosted by University of Arizona and Sandia National Labs
- Co-chair: "Thermofluids and Thermodynamics of Fluid Systems" at the 5th International Conference on Energy Sustainability, ASME, Washington DC 2011.

PUBLICATIONS

BOOKS AND BOOK CHAPTERS

- 1. Co-Editor with P.A. Deymier and Keith Runge, *Multiscale paradigms in integrated computational materials science and engineering, Springer* (2016)
- 2. Consistent Embedding Frameworks for Predictive Multi-theory Multiscale Simulations: Chapter in *Multiscale* paradigms in integrated computational materials science and engineering, Springer (2016) Krishna Muralidharan, K. Runge, P.A. Deymier
- 3. Interatomic Potentials Including Chemistry: Chapter in *Multiscale paradigms in integrated computational materials science and engineering, Springer* (2016) S.M. Valone, Krishna Muralidharan, K. Runge
- 4. Atomistic simulation methods: *SPIE/ASME handbook of nanotechnology (chapter 8), section: nanometer structure theory, modeling and simulation (2003)* P. A. Deymier, V. Kapila, Krishna Muralidharan
- 5. Nanoscale Phononic Crystals and Structures: Chapter 9 in *Acoustic metamaterials and phononic crystals* (ed. P. A. Deymier), Springer series in solid-state sciences, (2012) N. Swinteck, Krishna Muralidharan, P. Deymier, R. Erdmann

PEER-REVIEWED ARTICLES (AS INDEXED ON ISI-WEB OF KNOWLEDGE)

- 1. Huang, WJ, Bringuier S, Paul J, Potter K-S, Muralidharan K, Potter BG, "An atomistic assessment of the impact of flaw orientation on the elastic and failure behavior of single-crystal Si nanometre-thick slabs," Philosophical Magazine (2017) (http://dx.doi.org/10.1080/14786435.2017.1340686)
- 2. Ma D, Sandoval, S, Raghavan S, Muralidharan K, "Effect of surface preparation of copper on spin-coating driven self-assembly of fullerene molecules," Microelectronic Engineering, 170 8-15 (2017).
- 3. Weisbart C, Raghavan S, Muralidharan K, Potter BG, "Electrocoagulation driven fabrication of graphene oxide films" Carbon, 116 318-324 (2017)
- 4. Gur S, Bringuier S, Manga VR, Muralidharan K, Frantziskonis G, "Evolution of internal strain in austenite phase during thermally induced martensitic phase transformation in NiTi shape memory alloys" Computational Materials Science 133, 52-59 (2017)
- 5. Sadat MR, Bringuier S, Asaduzzaman A, Muralidharan K, Zhang, L, "A molecular dynamics study of the role of molecular water on the structure and mechanics of amorphous geopolymer binders," J. Chemical Physics, 145(13), 134706 (2016)
- 6. Pham D, Dycus JH, LeBeau JM, Manga VR, Muralidharan K, Corral E, "Processing Low-Oxide ZrB2 Ceramics with High Strength Using Boron Carbide and Spark Plasma Sintering," J. American Ceramic Society 99(8), 2585 (2016).
- 7. Dubus B, Swinteck N, Muralidharan K, Vasseur J, Deymier PA, "Nonlinear Phonon Modes in Second-Order Anharmonic Coupled Monoatomic Chains," J. Vibrations and Acoustics, 138(4) 041016 (2016).
- 8. Al-Sayoud AQ, Manga VR, Edwards AN, Deymier PA, Muralidharan K, Potter BG, Runge K, Lucas P, "Structure of ZnCl2 Melt. Part I: Raman Spectroscopy Analysis Driven by Ab Initio Methods," J. Physical Chemistry B, 120(17), 4174 (2016).
- 9. Asaduzzaman A, Runge K, Deymier PA, Muralidharan K, "The Role of Aluminum Substitution on the Stability of Substituted Polyhedral Oligomeric Silsesquioxanes," Zeitcshrift Fur Physikalische Chemie 230(S1), 1005 (2016).
- 10. Manga VR, Swinteck N, Bringuier S, Lucas P, Deymier P, Muralidharan K, "Interplay between structure and transport properties of molten salt mixtures of ZnCl2-NaCl-KCl: A molecular dynamics study," J. Chemical Physics, 144(9). 094501 (2016).
- 11. Sadat MR, Bringuier S, Asaduzzaman A, Muralidharan K, Zhang L, "An atomistic characterization of the interplay between composition, structure and mechanical properties of amorphous geopolymer binders," J. Noncrystalline solids, 434, 53(2016).
- 12. Bringuier S, Manga VR, Runge K, Deymier PA, Muralidharan K, An atomic scale characterization of coupled grain boundary motion in silicon bicrystals, PHILOSOPHICAL MAGAZINE Volume: 95 Issue: 36 Pages: 4118-4129 Published: DEC 22 2015
- 13. Deymier PA, Runge K, Swinteck N, Muralidharan K, Torsional topology and fermion-like behavior of elastic waves in phononic structures, COMPTES RENDUS MECANIQUE Volume: 343 Issue: 12 Pages: 700-711 Published: DEC 2015

- 14. Energetics of substituted polyhedral oligomeric silsesquioxanes: a DFT study, Asaduzzaman A, Runge K, Muralidharan K, Deymier PA, Zhang L, MRS COMMUNICATIONS Volume: 5 Issue: 3 Pages: 519-524 Published: SEP 2015
- Sridhar D, Balakrishnan K, Gnanaprakasa TJ, Raghavan S, Muralidharan K, Self-assembled fullerene additives for boosting the capacity of activated carbon electrodes in supercapacitors, RSC ADVANCES Volume: 5 Issue: 78 Pages: 63834-63838 Published: 2015
- 16. Bringuier S, Manga VR, Runge K, Deymier P, Muralidharan K, "Grain boundary dynamics of SiC bicrystals under shear deformation," MATERIALS SCIENCE AND ENGINEERING A Volume: 634 Pages: 161-166 Published: MAY 14 2015.
- 17. *Asaduzzaman A, Muralidharan K, Ganguly J, "Incorporation of water into olivine during nebular condensation: Insights from density functional theory and thermodynamics, and implications for phyllosilicate formation and terrestrial water inventory," METEORITICS & PLANETARY SCIENCE Volume: 50 Issue: 4 Pages: 578-589 Published: APR 2015
- 18. Gnanaprakasa TJ, Sridhar D, Zega T, Potter BG, Beck W, Runge K, Deymier PA, Raghavan S, Muralidharan K, "Graphene mediated self-assembly of fullerene nanorods," CHEMICAL COMMUNICATIONS Volume: 51 Issue: 10 Pages: 1858-1861 Published: JAN 2015.
- Gnanaprakasa TJ, Gu Y, Eddy SK, Han ZX, Raghavan S, Muralidharan K, "The role of copper pretreatment on the morphology of graphene grown by chemical vapor deposition," MICROELECTRONIC ENGINEERING Volume: 131 Pages: 1-7 Published: JAN 5 2015
- 20. *Asaduzzaman, A. M.; Zega, T. J.; Laref, Slimane, Runge K, Deymier P, Muralidharan K, "A computational investigation of adsorption of organics on mineral surfaces: Implications for organics delivery in the early solar system," EARTH AND PLANETARY SCIENCE LETTERS Volume: 408 Pages: 355-361 Published: DEC 15 2014
- 21. Guerder, Pierre-Yves; Deymier-Black, Alix C.; Swinteck, Nichlas Z, Muralidharan K, Vasseur J. Deymier P., "Multi-phonon scattering processes in one-dimensional anharmonic biological superlattices: Understanding the dissipation of mechanical waves in mineralized tissues," JOURNAL OF THE MECHANICAL BEHAVIOR OF BIOMEDICAL MATERIALS Volume: 37 Pages: 24-32 Published: SEP 2014
- 22. Trzaskowski, Bartosz; Adamowicz, Ludwik; Beck, Warren, Muralidharan K, Deymier P., "Exploring structures and properties of new geodesic polyarenes," CHEMICAL PHYSICS LETTERS Volume: 595 Pages: 6-12 Published: MAR 18 2014
- 23. Manga VR, Bringuier S, Paul J, Jayaraman S, Lucas P, Deymier PA, Muralidharan K, "Molecular dynamics simulations and thermodynamic modeling of NaCl-KCl-ZnCl2 ternary system" CALPHAD-COMPUTER COUPLING OF PHASE DIAGRAMS AND THERMOCHEMISTRY Volume: 46 Pages: 176-183 Published: SEP 2014.
- 24. Deymier PA, Swinteck N, Muralidharan K, Runge K, "Rotational modes in a phononic crystal with Fermion like behavior," JOURNAL OF APPLIED PHYSICS Volume: 115 Issue: 16 Article Number: 163510 Published: APR 28 2014
- 25. Laref, S, Cao J, Asaduzzaman A, Runge K, Deymier PA, Ziolkowski R, Miyawaki M, Muralidharan K, "Sizedependent permittivity and intrinsic optical anisotropy of nanometric gold thin films: a density functional theory study," OPTICS EXPRESS, 21(10), 11827-11838 (2013).

- 26. Campbell SD, Ziolkowski RW, Cao J, Muralidharan K, Deymier PA, "Anisotropic permittivity of ultra-thin crystalline Au films: Impacts on the plasmonic response of metasurfaces," APPLIED PHYSICS LETTERS 103(9), 091106 (2013).
- 27. Laref S, Asaduzzaman A, Beck W, Deymier PA, Runge K, Adamowicz L, Muralidharan K, "Characterization of graphene–fullerene interactions: Insights from density functional theory," CHEM. PHYS LETT (2013). http://dx.doi.org/10.1016/j.cplett.2013.07.033
- 28. Trzaskowski B, Adamowicz L, Beck W, Muralidharan K, Deymier PA, "Impact of Local Curvature and Structural Defects on Graphene–C60 Fullerene Fusion Reaction Barriers" J.PHYSICAL CHEMISTRY C (2013). DOI: 10.1021/jp405301e
- 29. Swinteck N, Muralidharan K, Deymier PA, "Phonon Scattering in One-Dimensional Anharmonic Crystals and Superlattices: Analytical and Numerical Study," J. VIBRATIONS AND ACOUSTICS-TRANSACTIONS OF ASME, 135, 041016 (2013)
- 30. *Vattuone L, Smeriri M, Savio L, Asaduzzaman AM, Muralidharan K, Rocca M, "Accretion disc origin of water," PHIL. TRANS. R. SOC. A, 371 20110585 (2013).
- 31. *Asaduzzaman A, Laref S, Runge K, Deymier PA, Cheng H-P, Drake MJ, Muralidharan K, "A first-principles characterization of water adsorption on forsterite grains," PHIL. TRANS. R. SOC. A, 371 20110582 (2013).
- 32. Proczka JJ, Muralidharan K, Villela D, Simmons JH, Frantziskonis G, "Guidelines for the pressure and efficient sizing of pressure vessels for compressed air energy storage," ENERGY CONVERSION AND MANAGEMENT Volume: 65 Special Issue: SI Pages: 597-605 DOI: 10.1016/j.enconman.2012.09.013 Published: JAN 2013
- 33. Muralidharan K, Erdmann RG, Runge K, Deymier PA, "Asymmetric energy transport in defected boron nitride nanoribbons: Implications for thermal rectification," AIP ADVANCES Volume: 1 Issue: 4 Article Number: 041703 DOI: 10.1063/1.3675924 Published: DEC 2011
- 34. Bringuier S, Swinteck N, Vasseur JO, Robillard JF, Runge K, Muralidharan K, Deymier PA, "Phase-controlling phononic crystals: Realization of acoustic Boolean logic gates," JOURNAL OF THE ACOUSTICAL SOCIETY OF AMERICA Volume: 130 Issue: 4 Pages: 1919-1925 DOI: 10.1121/1.3631627 Part: Part 1 Published: OCT 2011
- 35. Robillard JF, Bucay J, Deymier PA, Shelke A, Muralidharan K, Merheb B, Vasseur JO, Sukhovich A, Page JH, "Resolution limit of a phononic crystal superlens," PHYSICAL REVIEW B Volume: 83 Issue: 22 Article Number: 224301 DOI: 10.1103/PhysRevB.83.224301 Published: JUN 9 2011
- 36. Bringuier S, Swinteck N, Vasseur JO, Robillard JF, Runge K, Muralidharan K, Deymier PA, "Phase-controlling phononic crystal," APPLIED PHYSICS LETTERS Volume: 98 Issue: 10 (2011)
- 37. Robillard JF, Muralidharan K, Bucay J, Deymier PA, Beck W, Barker D, "Phononic Metamaterials for Thermal Management: An Atomistic Computational Study," CHINESE JOURNAL OF PHYSICS Volume: 49 Issue: 1 Special Issue: SI Pages: 448-461 Published: FEB 2011.
- 38. *de Leeuw NH, Catlow CRA, King HE, Putnis A, Muralidharan K, Deymier P, Stimpfl M, Drake MJ, "Where on Earth has our water come from?," CHEMICAL COMMUNICATIONS Volume: 46 Issue: 47 Pages: 8923-8925 DOI: 10.1039/c0cc02312d Published: 2010

- 39. Mishra SK, Deymier PA, Muralidharan K, Frantziskonis G, Pannala S, Simunovic S, "Modeling the coupling of reaction kinetics and hydrodynamics in a collapsing cavity," ULTRASONICS SONOCHEMISTRY Volume: 17 Issue: 1 Pages: 258-265 DOI: 10.1016/j.ultsonch.2009.05.014 Published: JAN 2010
- 40. Merheb B, Deymier PA, Muralidharan K, Bucay J, Jain M, Aloshyna-Lesuffleur M, Greger RW, Mohanty S, Berker A, "Viscoelastic effect on acoustic band gaps in polymer-fluid composites," MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING Volume: 17 Issue: 7 Article Number: 075013 DOI: 10.1088/0965-0393/17/7/075013 Published: OCT 2009
- 41. Bucay J, Roussel E, Vasseur JO, Deymier PA, Hladky-Hennion AC, Pennec Y, Muralidharan K, Djafari-Rouhani B, Dubus B, "Positive, negative, zero refraction, and beam splitting in a solid/air phononic crystal: Theoretical and experimental study," PHYSICAL REVIEW B Volume: 79 Issue: 21 Article Number: 214305 DOI: 10.1103/PhysRevB.79.214305 Published: JUN 2009
- 42. Sukhovich A, Merheb B, Muralidharan K, Vasseur JO, Pennec Y, Deymier PA, Page JH, "Experimental and Theoretical Evidence for Subwavelength Imaging in Phononic Crystals," PHYSICAL REVIEW LETTERS Volume: 102 Issue: 15 Article Number: 154301 DOI: 10.1103/PhysRevLett.102.154301 Published: APR 17 2009
- 43. *Muralidharan K, Stimpfl M, Deymier P, de Leeuw NH, Drake MJ, "Origin of water in the inner Solar System: A kinetic Monte Carlo study of water adsorption on forsterite," ICARUS Volume: 198 Issue: 2 Pages: 400-407 DOI: 10.1016/j.icarus.2008.07.017 Published: DEC 2008
- 44. Frantziskonis, G, Muralidharan, K., Deymier, P.; Simunovic, S, Nukala, P, Pannala, S, "Time-parallel multiscale/multiphysics framework," JOURNAL OF COMPUTATIONAL PHYSICS Volume: 228 Issue: 21 Pages: 8085-92 Published: 20 Nov. 2009
- 45. Mishra, S.K, Muralidharan, K, Pannala, S, Simunovic, S, Daw, C.S, Nukala, P, Fox, R, Deymier, P.A, Frantziskonis, G, "Spatiotemporal compound wavelet matrix framework for multiscale/multiphysics: case study of a heterogeneous reaction/diffusion system," INTERNATIONAL JOURNAL OF CHEMICAL REACTOR ENGINEERING Volume: 6 Pages: 43 pp. Published: 01 2008
- 46. Muralidharan K, Mishra SK, Frantziskonis G, Deymier PA, Naula P, Simunovic S, Pannala S, "Dynamic compound wavelet matrix method for multiphysics and multiscale problems," PHYSICAL REVIEW E Volume: 77 Issue: 2 Article Number: 026714 DOI: 10.1103/PhysRevE.77.026714 Part: Part 2 Published: FEB 2008
- 47. Mishra SK, Muralidharan K, Deymier PA, Frantziskonis G, Pannala S, Simunovic S,"Wavelet-Based Spatial Scaling of Coupled Reaction-Diffusion Fields," INTERNATIONAL JOURNAL FOR MULTISCALE COMPUTATIONAL ENGINEERING Volume: 6 Issue: 4 Pages: 281-297 Published: 2008
- 48. Muralidharan K, Torras J-T, Trickey SB, "Energetics and mechanical properties of silica nanotubes," JOURNAL OF PHYSICS-CONDENSED MATTER Volume: 19 Issue: 38 Article Number: 386238 DOI: 10.1088/0953-8984/19/38/386238 Published: SEP 26 2007
- 49. Torras J-T, He Y, Cao C, Muralidharan K, Deumens E, Cheng HP, Trickey SB, "PUPIL: A systematic approach to software integration in multi-scale simulations," COMPUTER PHYSICS COMMUNICATIONS Volume: 177 Issue: 3 Pages: 265-279 DOI: 10.1016/j.cpc.2007.01.009 Published: AUG 1 2007
- 50. Muralidharan K, Oh K-D, Deymier PA, Runge K, Simmons JH, "Molecular dynamics simulations of atomic-level brittle fracture mechanisms in amorphous silica," JOURNAL OF MATERIALS SCIENCE Volume: 42 Issue: 12 Pages: 4159-4169 DOI: 10.1007/s10853-007-1638-2 Published: JUN 2007

- 51. Muralidharan K, Cao C, Wan YX, Runge K, Cheng HP," Environment dependent dynamic charge potential for silica: Application to nanoscale silica structures," CHEMICAL PHYSICS LETTERS Volume: 437 Issue: 1-3 Pages: 92-98 DOI: 10.1016/j.cplett.2007.01.081 Published: MAR 22 2007
- Deymier PA, Oh KD, Muralidharan K, Frantziskonis G, Runge K, "Selection of domains for coarse and fine levels of description in mixed-potential simulations," JOURNAL OF COMPUTER-AIDED MATERIALS DESIGN Volume: 13 Issue: 1-3 Pages: 17-44 DOI: 10.1007/s10820-006-9013-1 Published: OCT 2006
- 53. Muralidharan K, Mallik A, Runge K, Deymier PA," Implementation of consistent embedding for a larger system Amorphous silica," JOURNAL OF COMPUTER-AIDED MATERIALS DESIGN Volume: 13 Issue: 1-3 Pages: 61-73 DOI: 10.1007/s10820-006-9015-z Published: OCT 2006
- 54. Cheng HP, Wang LL, Du MH, Cao C, Wan YX, He Y, Muralidharan K, Greenlee G, Kolchin A, "Quantum, classical, and multi-scale simulation of silica-water interaction: molecules, clusters, and extended systems," JOURNAL OF COMPUTER-AIDED MATERIALS DESIGN Volume: 13 Issue: 1-3 Pages: 161-183 DOI: 10.1007/s10820-006-9009-x Published: OCT 2006
- 55. Muralidharan K, Simmons JH, Deymier PA, Runge K, "Molecular dynamics studies of brittle fracture in vitreous silica: Review and recent progress," JOURNAL OF NON-CRYSTALLINE SOLIDS Volume: 351 Issue: 18 Pages: 1532-1542 DOI: 10.1016/j.inoncrysol.2005.03.026 Published: JUN 15 2005
- 56. Baskes MI, Muralidharan K, Stan M, Valone SM, Cherne FJ, "Using the modified embedded-atom method to calculate the properties of Pu-Ga alloys," JOM-JOURNAL OF THE MINERALS METALS & MATERIALS SOCIETY Volume: 55 Issue: 9 Pages: 41-50 DOI: 10.1007/s11837-003-0029-7 Published: SEP 2003
- 57. Muralidharan K, Deymier PA, Simmons JH, "A concurrent multiscale finite difference time domain/molecular dynamics method for bridging an elastic continuum to an atomic system," MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING Volume: 11 Issue: 4 Pages: 487-501 Article Number: DOI: 10.1088/0965-0393/11/4/306 Published: JUL 2003

TECHNICAL REPORTS

Simmons JH, Muralidharan K, University of Arizona Compressed Air Energy Storage, USDOE-DE-OE0000424 (2012)

INVENTION DISCLOSURES AND PROVISIONAL PATENTS

- 1. Graphene Derived and Chemically Modified Graphene Derived Carbon Fibers (UA, Invention Disclosure-17-186) Krishna Muralidharan, Srini Raghavan and B.G. Potter
- 2. Electrocoagulation driven fabrication of graphene oxide films and membranes (UA, Invention Disclosure 17-059) Clovis Weisbart, Srini Raghavan, Krishna Muralidharan, B.G. Potter
- 3. Fullerene-Graphene Based High Efficiency Supercapacitors (UA15-081), Krishna Muralidharan and Srini Raghavan
- 4. Substrate and Solvent Mediated Synthesis of Fullerene Self-assemblies (UA-15-073), Krishna Muralidharan, Srini Raghavan, Tony J Gnanaprakasa, Deepak Sridhar
- 5. High Temp Heat Transfer Fluids (250 C 1000 C) for Use in Energy Capture Systems (UA-14-042)
- 6. Provisional Patent Application No. 61/695080 was filed on 8/30/2012 for 2001-13838-prov, "Size-dependent Permittivity and Intrinsic Optical Anisotropy of Nanometric Gold Thin Films"

CONFERENCE PROCEEDINGS

1. ORIGIN OF WATER IN EARTH WITH HIGH D/H RATIO RELATIVE TO PROTOSOLAR NEBULA, AND AN EXPLANATION OF ITS SIMILARITY WITH THE ISOTOPIC RATIOS OF CARBONACEOUS

- CHONDRITES AND ASTEROID VESTA, Ganguly J, Asaduzzaman A, Muralidharan K, Meteoritics and Planetary Science, 51(S1),A277 (2016).
- 2. EXPERIMENTAL AND COMPUTATIONAL INVESTIGATION OF MICROCRACK BEHAVIOR UNDER COMBINED ENVIRONMENTS IN MONOCRYSTALLINE SILICON, Huang WJ, Bringuier S, Paull J, Potter KS, Muralidharan K, Potter BG, Proc. SPIE 9563, Reliability of Photovoltaic Cells, Modules, Components, and Systems VIII, 956308
- 3. SYNTHESIS AND DELIVERY OF AMINO ACIDS TO THE EARLY EARTH VIA SURFACE CATALYSIS: A COMPUTATIONAL STUDY, Asaduzzaman A, Muralidharan K, Zega TJ, Runge K, 45th Lunar and Planetary Science Conference (Article # 1467) 2014
- 4. NEW PLASMONIC MATERIALS IN VISIBLE SPECTRUM THROUGH ELECTRICAL CHARGING Cao J, Balachandran R, Keswani M, Muralidharan K, Laref S, Ziolkowski R, Runge K, Deymier P, Raghavan S, Miyawaki M, ," Proceedings of the SPIE The International Society for Optical Engineering, Volume: 8632 Pages:86321I (7 pp.) 2013
- 5. A COMPUTATIONAL EXPLORATION OF THE ATTACHMENT OF ORGANICS TO MINERALS, Asaduzzaman AM, Muralidharan K, Runge K, Zega TJ, 44th Lunar and Planetary Science conference, # 2884, 2013: Publisher: Lunar and Planetary Institute
- 6. HYDRATION KINETICS OF PERICLASE, Asaduzzaman AM, Muralidharan K, Ganguly, 44th Lunar and Planetary Science conference, # 2396, 2013: Publisher: Lunar and Planetary Institute
- 7. CHEMICAL PATHWAYS AND MECHANISMS OF WATER ADSORPTION ON OLIVINE GRAINS: EVIDENCE FOR WET ACCRETION OF EARTH, Asaduzzaman AM, Muralidharan K, METEORITICS & PLANETARY SCIENCE Volume: 47 Special Issue: SI Pages: A48-A48 Supplement: 1 Published: JUL 2012
- 8. FIRST-PRINCIPLES INVESTIGATION OF ADSORPTION OF ORGANIC MOLECULES ON PLANETARY MATERIALS, Asaduzzaman AM, Muralidharan K, Runge K, Zega TJ, METEORITICS & PLANETARY SCIENCE Volume: 47 Special Issue: SI Pages: A47-A47 Supplement: 1 Published: JUL 2012
- 9. ELECTRONIC STRUCTURE CALCULATIONS OF WATER ADSORPTION ON FORSTERITE GRAINS: IMPLICATIONS FOR PLANETARY WATER, Muralidharan K, Drake MJ, METEORITICS & PLANETARY SCIENCE Volume: 46 Special Issue: SI Pages: A170-A170 Supplement: 1 Published: JUL 2011
- 10. WATER IN THE INNER SOLAR SYSTEM: INSIGHTS FROM ATOMISTIC AND ELECTRONIC STRUCTURE CALCULATIONS, Muralidharan K, Stimpfl M, de Leeuw NH, Deymier PA, Runge K, Drake MJ, METEORITICS & PLANETARY SCIENCE Volume: 44 Pages: A136-A136 Supplement: S Published: JUL 200
- 11. CONSISTENT EMBEDDING: A MULTISCALE APPROACH TO BRITTLE FRACTURE, K. Runge, K. Muralidharan, and P.A. Deymier, Materials Science & technology 2011, Symposium on Nano- and Atomic-scale Fracture, Oct. 16-20, 2011 Columbus, Ohio.
- 12. SMALL-SCALE SCALABLE CAES SYSTEM WITH THERMAL MANAGEMENT, J.H.Simmons, K. Muralidharan, G. Frantziskonis, Y. Son, Electrical energy Storage Applications and Technologies, San Diego, October, 2011.
- 13. ATOMISTIC SIMULATIONS OF ADSORPTION OF WATER ONTO FORSTERITE AND FAYALITE PLANAR SURFACES, M. Stimpfl, Muralidharan K, de Leeuw N, Deymier PA, Runge K, Drake MJ, 41st Lunar and Planetary Science conference, # 2493, 2011: Publisher: Lunar and Planetary Institute

- 14. HIGH-EFFICIENCY COMPRESSED AIR ENERGY STORAGE SYSTEMS FOR STAND-ALONE PV PANELS, D. Villela, S. de Valle, M. Alvarez, Krishna Muralidharan, P. Deymier, G. Frantziskonis, IEEE Photovoltaics, Hawaii (2010)
- 15. SOME PERHAPS MOST WATER IN THE EARTH MUST RESULT FROM ADSORPTION ON TO GRAINS IN THE ACCRETION DISK,
 - K. Muralidharan, Stimpfl M. de Leeuw N. H. Deymier P. A. Runge K. Drake M. J, 41st Lunar and Planetary Science conference, # 1882, 2009: Publisher: Lunar and Planetary Institute
- 16. ADSORPTION AS A WATER DELIVERY SOURCE IN THE INNER SOLAR SYSTEM: A KINETIC MONTE CARLO STUDY, K. Muralidharan, P. A. Deymier, M. Stimpfl, M. J. Drake, 40th Lunar and Planetary Science conference, # 1882, 2008: Publisher: Lunar and Planetary Institute
- 17. WAVELET BASED SPATIAL SCALING OF COUPLED REACTION DIFFUSION FIELDS, S. K. Misra, Krishna Muralidharan, P. A. Deymier, , G. Frantziskonis, S. Pannala, S. Simunovic, Lecture Notes in Computer Science, ICCS-2008, 5102, 301-310, 2008
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- 20. EXPERIMENTAL AND SIMULATION INVESTIGATIONS OF ACOUSTIC CAVITATION IN MEGASONIC CLEANING, Krishna Muralidharan, M. Keswani, S. Raghavan, P. Deymier, F. Eschbach, A. Sengupta, Proc. of SPIE- V6517, Emerging Lithographic Technologies XI March 15 2007
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- 2. TRANSPORT AND STOKES-EINSTEIN BEHAVIOR IN MOLTEN MIXTURES OF NETWORK-FORMERS AND NETWORK-MODIFIERS, VR. Manga, N. Swinteck, S. Bringuier, P. Deymier, K. Muralidharan, TMS, Nashville, Feb 14-18, 2016.
- 3. AB INITIO MOLECULAR DYNAMICS STUDY OF SPECIATION IN ALCL3-ZNCL2-BASED NETWORK FORMING LIQUIDS,
 - VR. Manga, Abduljabar Alsayoud, S. Bringuier, P. Lucas, P. Deymier, K. Muralidharan, TMS, Nashville, Feb 14-18, 2016.
- 4. MECHANICALLY ROBUST, THERMALLY INSULATING LINING FOR UNDERGROUND MINES, Krishna Muralidharan, M. Momayez, SME, Phoenix, Feb 24-28, 2016
- 5. SURFACE MEDIATED SYNTHESIS OF RECONFIGURABLE SHAPE-SHIFTING NANOSCALE TO MICROSCALE FULLERENE SELF-ASSEMBLIES FOR ENERGY APPLICATIONS,
 - S. Sandoval, Tony J. Gnanaprakasa, Dongni Ma, P. Deymier, Srini Raghavan, Krishna Muralidharan, MRS Spring Meeting, Phoenix, Mar 28-Apr 1, 2016.
- 6. ENVIRONMENT DEPENDENT DYNAMIC CHARGE POTENTIAL, Abduljabar Al-Sayoud, K. Runge, P. Deymier, Krishna Muralidharan, (poster), MRS Spring Meeting, Phoenix, Mar 28-Apr 1, 2016.
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- 8. EFFECT OF SURFACE PREPARATION OF COPPER ON SELF-ASSEMBLY OF FULLERENE MOLECULES,
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- 9. AN ENVIRONMENT DEPENDENT DYNAMIC CHARGE INTERATOMIC POTENTIAL FOR MODELING NANO AND BULK SILICA POLYMORPHS, Krishna Muralidharan, K. Runge, GOMD 2016, Madison, May 22-26 2016.
- 10. COMPUTATIONAL MODELING OF SYNTHESIS OF AMORPHOUS SERPENTINE FROM OLIVINE: IMPLICATIONS FOR PLANETARY WATER DELIVERY AND FORMATION OF HYDROUS MINERALS IN THE SOLAR NEBULA, Abu Asaduzzaman, Krishna Muralidharan, J Ganguly, GOMD 2016, Madison, May 22-26 2016.
- 11. ELECTROCHEMICAL SYNTHESIS OF MULTIFUNCTIONAL GRAPHENE OXIDE FILMS, Clovis Weisbart, Srini Raghavan, Krishna Muralidharan, B.G. Potter, MS&T, Salt Lake City, Oct 23-27 2016

- 12. MOLECULAR DYNAMICS STUDIES OF VISCOSITY AND THERMAL CONDUCTIVITY OF NACL-KCL-ZNCL2 MELTS,
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- 13. STRUCTURAL CHARACTERIZATION OF ZNCL2 BASED MOLTEN SALTS USING RAMAN SPECTROSCOPY AND QUANTUM CHEMICAL METHODS,
 - **VR. Manga**, A. Al-Sayoud, S. Bringuier, P. Lucas, P. Deymier, K. Muralidharan, 144th Annual TMS meeting, Orlando, March 2015
- 14. ANISOTROPY IN THE TRANSFORMATION DYNAMICS OF AUSTENITE (B2) TO MARTENSITE (B19') ASSOCIATED WITH SUPERELASTICITY IN NITI,
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- 16. THEORETICAL AND EXPERIMENTAL INVESTIGATIONS OF NANOMETRIC ALKALI OXIDE LAYERS ON SILICON AS LOW WORK FUNCTION ELECTRODES FOR THERMIONIC CONVERTERS.
 - A. Asaduzzaman, F. Morini, V. Giorgis, E. Dubois, J-F. Robillard, P. Deymier, **K. Muralidharan**, , 144th Annual TMS meeting, Orlando, March 2015
- 17. GRAPHENE SUBSTRATE MEDIATED SELF-ASSEMBLY OF ALIGNED FULLERENE NANORODS.
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- 18. COHERENT THERMAL PHONONS IN Si-Ge NANOSCALE PHONONIC CRYSTALS, N. Swinteck, **K. Muralidharan**, P. Deymier, European-MRS meeting, Lille, France, May 2014
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- 20. THERMODYNAMIC MODELING MIXED IONIC SYSTEMS,
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- 21. STRUCTURE AND THERMODYNAMICS OF MOLTEN SALT MIXTURES, **VR. Manga**, S. Bringuier, J. Paul, S. Jayaraman, P. Lucas, P. Deymier, K. Muralidharan, 143rd Annual TMS meeting, San Diego, 02/16-02/20/14
- 22. ENVIRONMENT DEPENDENT DYNAMIC CHARGE POTENTIALS (EDD-Q): A HIERARCHICAL APPROACH FOR ATOMISTIC MODELING OF CLUSTERS TO SOLIDS, **K. Muralidharan**, K. Runge, PA. Deymier,143rd Annual TMS meeting, San Diego, 02/16-02/20/14

- 23. SYNTHESIS AND DELIVERY OF AMINO ACIDS TO THE EARLY EARTH VIA SURFACE CATALYSIS: A COMPUTATIONAL STUDY (*POSTER*),
 - **AM. Asaduzzaman**, K. Runge, TJ. Zega, K. Muralidharan, 45th Lunar and Planetary Science Conference, Houston, 03/17-03/21/14
- 24. THE ROLE OF COPPER PRE-TREATMENT ON THE MORPHOLOGY OF GRAPHENE GROWN BY CHEMICAL VAPOR DEPOSITION,
 - **TJ. Gnanaprakasa**, Y. Gu, SK. Eddy, Z.Han, W. Beck, K. Muralidharan, S. Raghavan, SEMATECH Surface Preparation and Cleaning Conference, Austin, 04/22-04/24/14
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- 26. HYDRATION KINETICS OF PERICLASE: QUANTUM CHEMICAL CALCULATIONS AND IMPLICATIONS FOR THE TIMESCALE OF FORMATION OF THE SOLAR NEBULA (*POSTER*), AM. Asaduzzaman, K. Muralidharan, J. Ganguly, 44th Lunar and Planetary Science Conference, Houston, 03/05-03/10/13
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 K. Muralidharan, PA, Deymier, K. Runge, LAMMPS Users' Workshop and Symposium Series, 2013, Albuquerque, 08/08/13
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- 30. MECHANICAL FAILURE IN SIC BICRYSTALS, S. Bringuier, VR. Manga, P. Deymier, K. Muralidharan, MS&T, 2013, Montreal, Canada 11/1/13
- 31. MOLECULAR ASSEMBLY OF GRAPHENE/FULLERENE NANOSTRUCTURES, **TJ. Gnanaprakasa**, W. Beck, BG. Potter, K. Runge, P. Deymier, K. Muralidharan, MS&T, 2013, Montreal, Canada 11/1/13
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- 34. METALLIC THIN FILMS WITH TUNABLE OPTICAL PROPERTIES (*POSTER*), **K. Muralidharan**, S. Laref, J. Cao, K. Runge, P. Deymier, R. Ziolkowski, M. Miyawaki, MRS Fall meeting, Nov 24-29 2012, Boston, MA

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- WET ACCRETION OF EARTH: EXPERIMENTAL AND THEORETICAL EVIDENCE
 K. Muralidharan, A. Asaduzzaman, Institute for planets and exoplanets (IPLEX) at UCLA, Los Angeles, CA, 06/12-06/13/12
- 37. TWO-DIMENSIONAL MATERIALS WITH TUNABLE THERMAL PROPERTIES **K. Muralidharan**, R. Erdmann, P.A. Deymier and K. Runge, "MRS Fall meeting, Symposium W: Phonons in Nanomaterials—Theory, Experiments, and Applications, Nov.28-Dec. 2, 2011, Boston.
- 38. ACCRETION DISK ORIGIN OF EARTH'S WATER: LABORATORY EXPERIMENTS
 L. Vattuone, **K. Muralidharan**, M. Rocca, M.J. Drake, 74th Annual meeting of the Meteoritic Society,
 : Greenwich, England, August, 2011
- 39. ATOMISTIC AND ELECTRONIC STRUCTURE CALCULATIONS OF WATER ADSORPTION ON FORSTERITE GRAINS: IMPLICATIONS FOR PLANETARY WATER (INVITED) K. Muralidharan, M.J. Drake, The Royal Society Meeting on Surface Science in the Interstellar Medium, Kavli Royal Society International Centre at Chicheley Hall, England, 11th March 2011
- 40. WATER IN THE INNER SOLAR SYSTEM: INSIGHTS FROM ATOMISTIC AND ELCTRONIC-STRUCTURE CALCULATIONS (*POSTER*) Krishna Muralidharan, K. Runge, N. H. De Leeuw, P. A. Deymier, M. J. Drake Presented at 72nd Annual Meeting of the Meteoritical Society, July 13-18, 2009, Nancy, France
- 41. COMPRESSED AIR ENERGY STORAGE SYSTEMS FOR STAND-ALONE OFF-GRID PHOTO-VOLTAIC MODULES
 - D. Villela, S. Ashok, Krishna Muralidharan, P. A. Deymier Presented at Solar Fusion Day, University of Arizona, Aug, 2009, Tucson, AZ
- 42. SOME-PERHAPS MOST WATER IN THE EARTH MUST RESULT FROM ADSORPTION ON TO GRAINS IN THE ACCRETION DISK Krishna Muralidharan, P. A. Deymier, M. Stimpfl, N. H. de Leeuw, M. J. Drake Poster Presentation at Lunar and Planetary Science Conference, Mar 23-27, 2009, Woodlands, TX
- 43. A COMPUTATIONAL STUDY OF WATER ADSORPTION ON TO FORSTERITE GRAINS, **Krishna Muralidharan**, P. A. Deymier, M. Stimpfl, N. H. de Leeuw, M. J. Drake Presented at Surface and Interface Processes at the Molecular Level Aug, 2008, Lucca, Italy
- 44. ADSORPTION AS A WATER DELIVERY SOURCE IN THE INNER SOLAR SYSTEM: A KINETIC MONTE CARLO STUDY (*POSTER*), Krishna Muralidharan, P. A. Deymier, M. Stimpfl, M. J. Drake Poster Presentation at Lunar and Planetary Science Conference, Mar 10-14, 2008, League City, TX
- 45. WATER IN THE INNER SOLAR SYSTEM: A KINETIC MONTE CARLO STUDY **Krishna Muralidharan**, P. A. Deymier, M. Stimpfl, N. H. De Leeuw, M. J. Drake Presented at 70th Annual Meeting of the Meteoritical Society, Aug. 13-17, 2007, Tucson, AZ

46. FUNDAMENTAL PROCESSES IN MEGASONIC-IRRADIATED FLUIDS: APPLICATIONS TO CLEANING,

Krishna Muralidharan, Presented at SRC/SEMATECH Engineering Research Center for Environmentally Benign Semiconductor Manufacturing, Tucson AZ, 2007

47. ENVIRONMENT DEPENDENT DYNAMIC CHARGE POTENTIAL FOR SILICA L. Kemper, **Krishna Muralidharan**, Y. Wan, H. P. Cheng Presented at American Physical Society Annual March Meeting, Mar 11-17, 2006, Baltimore, MD

48. SIMULATION STUDIES OF MECHANICAL PROPERTIES OF NOVEL SILICA NANOSTRUCTURES

Krishna Muralidharan, J. Torras-Costa, S. B. Trickey

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49. A NEW CHARGE-TRANSFER POTENTIAL FOR SILICA

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50. DYNAMIC CHARGE POTENTIAL FOR WATER

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51. DYNAMICS OF BRITTLE FRACTURE IN SILICA GLASS: A LOOK AT STRUCTRUAL REARRANGEMENT MECHANISMS

Krishna Muralidharan, J. H. Simmons, P. A. Deymier

Presented at M. C. Weinberg Symposium, Journal of Non-Crystalline Materials, October 21-23, 2003, Tucson, AZ

52. MODELING BRITTLE FRACTURE IN VITREOUS SILICA: A MULTISCALE QM-MD APPROACH **Krishna Muralidharan**, J. H. Simmons, P. A. Deymier

Presented at Glass and Optical Materials Division Fall Meeting, American Ceramic Society, October 2003, Corning, NY

53. ATOMISTIC MODELING OF THE PHASE STABILITY IN THE Pu-Ga SYSTEM **Krishna Muralidharan**, M. I. Baskes, Marius Stan and S.G. Srinivasan Presented at 2003 Minerals, Metals and Materials Society Spring Meeting, March.2-6, 2003, San Diego, CA

54. MULTISCALE MODELING OF WAVE PROPAGATION: FDTD/MD HYBRID METHOD **Krishna Muralidharan**, P. A. Deymier, and J. H. Simmons Presented at 2002 Materials Research Society Spring Meeting, Apr.1-5, 2002, San Francisco, CA

55. LOCAL STABILITY OF INTERFACES BETWEEN DIFFERENT SIZED ATOMS **Krishna Muralidharan** and M.I. Baskes

Poster Presentation at Local and Nanoscale Structure in Complex Systems, Jan.27, 2002, Santa Fe NM

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- 2. ORIGIN OF WATER IN EARTH WITH HIGH D/H RATIO RELATIVE TO PROTOSOLAR NEBULA, AND AN EXPLANATION OF ITS SIMILARITY WITH THE ISOTOPIC RATIOS OF CARBONACEOUS CHONDRITES AND ASTEROID VESTA.
 - J. Ganguly, A. Asaduzzaman, K. Muralidharan, 7^{9th} Annual Meeting of the Meteoritic Society, Berlin 7-11 Aug 2016
- 3. INCORPORATION OF WATER IN PYROPE, VR Manga, M. Mookherjee, K. Muralidharan, AGU meeting, San Francisco, Dec 2014
- 4. ACCRETION DISK ORIGIN OF WATER.
 - Vattuone L, Smeriri M, Savio L, Muralidharan K, Rocca M, 19th International Vacuum congress, Paris France, 09/09/13
- NEW PLASMONIC MATERIALS IN VISIBLE SPECTRUM THROUGH ELECTRICAL CHARGING Jiangrong Cao, Rajesh Balachandran, Manish Keswani, Krishna Muralidharan, Slimane Laref, Richard W. Ziolkowski, Keith Runge, Pierre A. Deymier, Srini Raghavan, Mamoru Miyawaki SPIE Photonics West, San Francisco, Feb 2-7 2013
- 6. CONSISTENT EMBEDDING: A MULTISCALE APPROACH TO BRITTLE FRACTURE,
 - **K. Runge**, K. Muralidharan, and P.A. Deymier, Materials Science & technology 2011, Symposium on Nano- and Atomic-scale Fracture, Oct. 16-20, 2011 Columbus, Ohio.
- 7. SMALL-SCALE SCALABLE CAES SYSTEM WITH THERMAL MANAGEMENT,
 - **J.H.Simmons**, K. Muralidharan, G. Frantziskonis, Y. Son, Electrical energy Storage Applications and Technologies, San Diego, October, 2011.
- 8. PHONONIC CRYSTALS WITH COMPLETE PHASE SPACE PROPERTIES.
 - **P.A. Deymier**, J. Bucay, J-F. Robillard, K. Muralidharan, B. Merheb, J.O Vasseur, A. Sukhovich, J.H. Page, Y. Pennec, B. Djafari-Rouhani, L. Dobrzynski, A-C Hladky, B. Dubus, N. Swinteck, S. Bringuier, H. Chandra, A. Khelif, Phononics 2011, Santa Fe, May 29-June 2, 2011.
- 9. PHASE-CONTROLLING PHONONIC CRYSTAL,
 - **N. Swinteck**, S. Bringuier, P.A. Deymier, K. Runge, K. Muralidharan, J.O. Vasseur, Phononics 2011, Santa Fe, May 29-June 2, 2011
- 10. ACOUSTIC MATERIALS: NEGATIVE, POSITIVE AND ZERO REFRACTION AND SUPER-LENSING IN PHONONIC CRYSTALS
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- 11. ACOUSTIC METAMATERIALS: NEGATIVE, POSITIVE AND ZERO-ANGLE REFRACTION AND SUPERLENSING IN ACOUSTIC CRYSTALS
 - **P. A. Deymier**, J. Bucay, B. Mehreb, Krishna Muralidharan, Alexey Sukhovich3, John Page3, J. Vasseur, A.C. Hladky-Hennion, Y. Pennec, B.Jafari-Rouhani, B.Dubus and E.Roussel 2009 Materials Research Society Fall Meeting, Nov30-Dec 3, 2009, Boston, MA
- 12. PECULIAR REFRACTION PHENOMENA IN A SOLID/AIR PHONONIC CRYSTAL **J. O. Vasseur**, J. Bucay, E. Roussel, P. A. Deymier, Y. Pennec, A-C. Hladky-Hennion, K. Muralidharan, B. Djafari-Rouhani, B. Dubus
 - Presented at IEEE International Ultrasonics, 2009, Rome, Italy
- 13. WAVELET BASED SPATIAL SCALING OF COUPLED REACTION DIFFUSION FIELDS

- S. K. Misra, Krishna Muralidharan, P. A. Deymier, , G. Frantziskonis, S. Pannala, **S. Simunovic** International Conference on Computational Science (ICCS), June 23-25, 2008, Krakow, Poland
- 14. PARALLEL-IN-TIME MULTISCALE/MULTIPHYSICS FRAMEWORK G. Frantziskonis, Krishna Muralidharan, P. A. Deymier, S. Pannala, S. Simunovic International Conference "Scientific Computing to Computational Engineering, 3rd IC-SCCE, July 2008, Athens, Greece
- 15. REVERSIBLE AND DIRECTIONAL SELF-ASSEMBLY OF BIO-MOLECULAR TEMPLATES FOR NANOTECHNOLOGY INTERCONNECTS (**POSTER**)

Michele Pavanello, Krishna Muralidharan

Poster Presentation at 2007 National Science Foundation (NSF) Conference on International Research and Education in Engineering, Oct 30-Nov 1, 2007, Purdue University, West Lafayette, IN

- EFFECT OF SOLUTION CHEMISTRY IN MEGASONIC CLEANING
 M. Keswani, S. Raghavan, S. Verhaverbeke, Krishna Muralidharan, P. Deymier
 Presented at Surface Preparation and Cleaning Symposium SEMATECH, Austin 2007.
- 17. EXPERIMENTAL AND SIMULATION INVESTIGATIONS OF ACOUSTIC CAVITATION IN MEGASONIC CLEANING

Krishna Muralidharan, M. Keswani, S. Raghavan, P. Deymier, F. Eschbach, A. Sengupta Presented at SPIE, Emerging Lithographic Technologies XI March 15 2007, Santa Clara, CA

- 18. MULTISCALE MODELING OF FRACTURE IN SIO₂
 - **A. Mallik**, Krishna Muralidharan, K. Runge, J. W. Dufty Presented at South-Eastern Section of the American Physical Society, Nov 9-11, 2005, Gainesville, FL
- 19. SOFTWARE FOR INTEGRATIONOF QUANTUM MECHANICAL AND QUANTUM REGIONS IN MOLECULAR DYNAMICS
- **J. Torras**, Krishna Muralidharan, E. Deumens, S. B. Trickey

Presented at International Society for Theoretical Chemical Physics, July 20-25, 2005, New Orleans, LA

- 20. CHOOSING A POTENTIAL FOR MULTISCALE MODELING
- **A. Mallik**, Krishna Muralidharan, K. Runge, J. W. Dufty

Presented at American Physical Society Annual March Meeting, Mar. 21, 2005, Los Angeles, CA

- 21. PHASE STABILITY OF Pu-Ga ALLOYS FROM FIRST-PRINCIPLES AND MOLECULAR DYNAMICS CALCULATIONS
- M. A. Stan, M. I. Baskes, Shao-Ping Chen, and Krishna Muralidharan

Presented at CALPHAD XXXII International Conference on Phase Diagram Calculations and Computational Thermochemistry, May 25-30, 2003, La Malbaie, Quebec, Canada

22. PHASE STABILITY IN THE Pu-Ga SYSTEM FROM FIRST PRINCIPLES AND MOLECULAR DYNAMICS CALCULATIONS

Marius Stan, M. I. Baskes, and Krishna Muralidharan

Presented at 2003 Materials Research Society Fall Meeting, Dec. 1-5, 2003, Boston, MA

COLLOQUIA/SEMINARS

1. EXPERIMENTAL AND THEORETICAL INVESTIGATIONS OF GRAPHENE-FULLERENE BASED SYSTEMS FOR TECHNOLOGICAL APPLICATIONS,

Krishna Muralidharan, Department of Physics Seminar, IIT Madras, Chennai, December 27th 2016.

2. GRAPHENE AND FULLERENE ADDITIVES FOR ENHANCING PERFORMANCE OF CARBON SUPERCAPACITORS

Krishna Muralidharan, Invited lecture at IEMN, Lille, May 2015

- 3. GRAPHENE-FULLERENE BASED SYSTEMS FOR TECHNOLOGICAL APPLICATIONS Krishna Muralidharan, Invited lecture at IEMN, Lille, June 2014
- 4. A BOTTOM-UP APPROACH TO MULTISCALE MODELING OF MATERIALS Krishna Muralidharan, Department Seminar, CEEM, University of Arizona, Nov 2013
- 5. DELIVERY OF WATER AND ORGANICS TO EARLY EARTH: INSIGHTS FROM QUANTUM CHEMISTRY

Krishna Muralidharan, LPLC 2013, Tucson, 08/23/13

- SMALL SCALE COMPRESSED AIR ENERGY STORAGE SYSTEMS
 Krishna Muralidharan, Department Seminar, Materials Science and Engineering, University of Arizona, March 2011
- 7. MULTISCALE MODELING OF MATERIALS Krishna Muralidharan, Department Seminar, Applied Math, University of Arizona, Nov 2010
- 8. NOVEL PHONONIC METAMATERIALS FOR ACOUSTIC AND THERMAL APPLICATIONS
 Krishna Muralidharan, SRC Engineering Research Center for Environmentally Benign Semiconductor
 Manufacturing (ERC) Seminar Series, March 2010
- ENVIRONMENT DEPENDENT DYNAMIC CHARGE POTENTIALS: APPLICATIONS TO WATER AND SILICA Krishna Muralidharan, Presented at Quantum Chemistry Laboratory, University of Warsaw, Poland, June, 2007
- FUNDAMENTAL PROCESSES IN MEGASONIC-IRRADIATED FLUIDS: APPLICATIONS TO CLEANING Krishna Muralidharan, SRC Engineering Research Center for Environmentally Benign Semiconductor Manufacturing (ERC) Seminar Series, April 2007
- 11. BRITTLE FRACTURE IN AMORPHOUS SILICA
 Krishna Muralidharan, Department Seminar, Quantum Theory Project, University of Florida, Nov 2004
- 12. ATOMISTIC CHARACTERIZATION OF FAILURE MECHANISMS IN AMORPHOUS SILICA Krishna Muralidharan, Department Seminar, Department of Physics and Astronomy, University of New Mexico, Jan 2004

GRANTS AND CONTRACTS (FUNDED)

I have received research contracts from different federal agencies as well as funding from industry. The cumulative funding of all the research grants that I have been involved with exceeds \$ 14 million, out of which my direct share is approximately \$ 3 million.

Principal Investigator projects							
agency	agency Years Title/Topic Funding Important contributions Publications/pro Collabora						
			(\$)		ducts	S	
NASA	2011-	Primordial	240,000	A new hypothesis on the	6 papers,	LPL	
	2014	Differentiation of		endogenous origin of water			

		1	1	18		1
		the Terrestrial		and organics. Recent	5 conf.	
		planets/Origin of		discovery of water on other	presentation	
		water and organics		rocky planets concur our		
		on Earth		findings		
Canon	2011-	Metallic Thin	450,000	The first demonstration of	3 papers	ECE, Opt.
	2013	Films with		optically tunable metallic	2 provisional	Sci
		Tunable		devices for hyperspectral	patents	
		Permittivity/		applications	2 conference	
		Optical			presentation	
		Metamaterials				
NSF	2011-	Fabrication and	150,000	The first demonstration of	5 papers	Physics,
	2013	characterization		surface mediated self-	3 conference	Chem.
		of a 3D Carbon		assemblies of fullerenes	presentation	
		Nanostructure-			1 PhD	
		Mattressene				
		/Carbon				
		nanostructures				
Raytheon	2011-	Engineering	367,000	A new modeling paradigm	ITAR-protected	CEEM
	2018	Strength of ZnS	consolid	for scale-free modeling of	data, 1	
		/Mechanics of	ated	materials	conference	
		nanocrystalline	over		presentation	
		ceramics	multiple			
			projects			
REN	2013-	Graphene	60,000	First demonstration of	2 papers,	
(UA)	2014	mediated self-		fullerene based	2 conference	
		assembled		supercapacitors; high	presentation	
		fullerene		efficiency, low-cost	2 invention	
		nanotubes for		alternatives to graphene	disclosure	
		ultracapacitor		based systems	1 M.S	
		applications				
		/Supercapacitor				
Amazon	2014-	Mechanical and	10,000	Parallelizable molecular	1 conference	
	2015	fracture		dynamics software	presentation	
		properties of				
		ceramics				
		/Computational				
	1	software				

Co-Principal Investigator projects							
DOE	2012-	Halide and Oxy-	5.5	Identification of salt	4 papers,	AME, CHEE,	
	2017	Halide Eutectic	Million	compositions via	12 conference	Mining,	
		Systems for High		computational means to	presentations		
		Performance High		inform experiments	1 invention		
		Temperature Heat			disclosure		
		Transfer					
		Fluids/High					
		efficiency thermal					
		fluids for					
		concentrated solar					
		plants					
NASA	2013-	Asteroidal and	480,000	Unequivocally shown	2 paper,	Geosciences	
	2016	Early Solar		that the timescale of			

		Cristons		hydrous phyllosiliaeta	1 conforces	
		System		hydrous phyllosilicate	4 conference	
		Processes:		formation is well within	presentations	
		Theoretical,		the time-scale of planet		
		Experimental		formation, disproving		
		and		previous hypothesis		
		Observational				
		Studies of				
		Mineralogical				
		Records in				
		Meteorites/Time				
		scale of planetary				
		formation				
NASA	2015-	Earth in other	5.7	Important insights into	1 paper,	Steward, LPL
1111011	2019	solar systems:	Million	organics incorporation in	3 conference	Steward, Er E
	2017	towards forming	William	planetary building blocks	presentations	
		and discovering		planetary building blocks	presentations	
		planets with				
		biocritical				
		ingredients				
		/Search for new				
177.0 0		habitable planets				2.51
NIOSH	2014-	Innovative	1.2	Using computational	3 paper	Mining,
	2019	Solutions for	Million	methods, identified	5 conference	Public Health
		Heat		structure composition of	presentation	
		Management in		thermal insulating		
		Hot		barriers		
		Underground				
		Mines:				
		Ventilation				
		Research and				
		Capacity				
		Buildings/ Non-				
		toxic thermal				
		coatings for mine-				
		walls derived				
		from waste				
		· ·				
Tr. 4	2011	materials	212.000	D 4 4 1 5 4 5 4	2	
Toyota	2011-	Nanophononic	213,000	Demonstrated for the first	3 papers	
	2013	Crystals for		time the presence and		
		Thermal Control		role of rotational modes		
		/Thermal		in determining thermal		
		interface		and phonon response of		
		materials, phonon		materials		
		metamaterials				
DOE/SFAz/	2009-	Critical	1.67	Demonstrated for the first	3 papers,	SIE, CEEM
AzRISE	2013	Components of	Million	time that CAES can be	4 conference	
		Energy Storage		scaled well for small	proceedings,	
		/Compressed-air		scale (10 kW) and	1 technical	
		energy storage		medium scale (100kW-	report,	
		(CAES)		1MW) applications	1 invention	
		(=====/		,pp	disclosure	
					1 M.S	
]				1 101.0	

Partnership	2011-	FACE –	155,000	New carbon	2 conference	Opt. Sci
University	2015	Advanced		nanostructures for	presentations	
Fund (PUF)		Materials for		thermal and optical		
		Energy and		applications		
		Optics/new				
		multifunctional				
		materials				

RESEARCH SUPERVISION and MENTORSHIP

Postdoctoral Associates

- Abu Asaduzzaman (2011-2016)
- Slimane Laref (2011-2013)
- Venkateswara Rao Manga (2013-2016)
- Sahila Perananthan (2017-present)
- Ali Abbaspour Tamijani (2017).

Graduate Students

- Pratish Rao (PhD): Dec, 2018 (expected date of graduation)
- Clovis Weisbart (PhD): May, 2018 (expected date of graduation)-joint supervision with Dr. B.G. Potter
- Abduljabar Al-Sayoud (PhD): Dec, 2017 (expected date of graduation)-joint supervision with Dr. Pierre Deymier
- Matthew Rand (M.S): May, 2018 (expected date of graduation)
- Ben Geller (M.S): May, 2018 (expected date of graduation)
- Tony Jefferson Gnanaprakasa (PhD)-graduated in 2015. "Surface engineering and synthesis of graphene and fullerene nanostructures"
- Stefan Bringuier (PhD) –graduated in 2015. "Mechanical properties of symmetric tilt grain boundaries in silicon and silicon carbide: A molecular dynamics study"
- Deepak Sridhar (M.S)-graduated in 2015. "Carbon nanostructures based supercapacitors."
- Vijayanathan Kasinathan Veerasamy (M.S)-graduated in 2013. "Thermal management in small scale compressed air energy storage systems."

Capstone Project advisor

- Kurumi Austin (B.S. 2017)
- Josh Vita (B.S 2017)
- Jared Jensen (B.S 2016)
- Mike Dokouzian (B.S 2016)
- Ben Geller (B.S. 2016)
- Wilson Kong (B.S, 2015)
- Steve Kyle Eddy (B.S, 2014)
- Stephen Purdy (B.S, 2012)

<u>Undergraduate Research Mentor (funded via research grants)</u>

- Conor O Neill (B.S. 2018)-expected date of graduation
- Daniel Molina Escalante (B.S. 2018)-expected date of graduation
- Christopher Tang (B.S. 2017)
- Jillian Grass (B.S. 2017)
- Ben Geller (B.S 2016)
- Eric Gabriel (B.S, 2016)
- Tarlton Ferrin (B.S, 2016)
- Matthew Jordan (B.S, 2015)
- Joshua Paul (B.S 2015)

- Sean Athanasios Katsarelis (B.S, 2012)
- Alex Bergdahl (B.S, 2012)
- Christopher Mendoza (B.S, 2013)
- Eric Gabriel (B.S, 2016)
- Tarlton Ferrin (B.S, 2016)
- Dominique Villela (B.S, 2011)
- Ryan Decker (High school student)

Research Experience for Undergraduates (REU) students

- Kathleen Van Atta (2017)
- Yen Do-Thien (2017)
- Daniel Escalante (2016)
- Christian Bartholomew (2015)

DISSERTATION/THESIS COMMITTEE

- Sourav Gur (PhD)
- Dongni Ma (PhD)
- Wei-Jie Huang (PhD)
- Mellia Oana-Jana (PhD)
- David Pham (PhD)
- Mark Lauer (PhD)
- Pierre Yves Guerder (PhD)
- Ozgur Gulbiten (PhD)
- Russell Beal (PhD)
- Rajkumar Govindarajan (PhD)
- Dinesh Thanu (PhD)
- Luke Walker (PhD)
- Sangita Kumari (PhD)
- Jenny Taubert (PhD)
- Darrick M Buban (PhD)
- N. Swinteck (PhD)
- Paul Neff (M.S)
- Chrishani Lidamulage (M.S)
- Shanna Tunne (M.S)
- Robert Schultz (M.S)
- Dominique Villela (M.S)
- JJ Prozcka (M.S)
- C. Swanborg (MS)
- S. de Valle (MS)
- J. Long (MS)
- M. Alvarez (MS)