DR. AMITAVA MOITRA

Assistant Professor
Department of Physics
Raidighi College

Research Area: Integrated Computational Materials Engineering (ICME)

Major Career Achievements:

Knowledge transfer through theory development in 1) **formability theory** on how to increase room temperature ductility in magnesium and its alloys (**Moitra's Order of Formability (MOF)**: http://journals.iop.org/cws/article/jpcm/58851), and 2) **alloy design** for industrial control on alu-minum solid solution concentration in magnesium for predictive structural behavior for magnesium alloys (**Fundamental Research Award, Light Metals Division, The Minerals, Metals, and Materials Society, 2012**).

Academic Preparations

Doctor of Philosophy, Applied (Engineering) Physics
4.0 GPA, courses are taken from three academic departments in MSU

Dissertation Title: Magnetic, mechanical, and thermal properties of materials using density functional theory and semiempirical methods.
Bagley College of Engineering, Mississippi State University, Feb., 2010.

Master of Science, Physics
Department of Physics and Astronomy, Mississippi State University, December, 2007.

Master of Science, Electronic Science
Jadavpur University, Kolkata, India, July 2002
Dissertation: Traffic and Streetlight Controller.

Bachelor of Science, Physics (Honours)
University of Calcutta, Kolkata, India, Aug. 2000.

Experiences

Assistant Professor
Department of Physics, Raidighi College, University of Calcutta, Since June, 2017.

Marie Curie (AMAROUT) Fellow and Senior Associate IMDEA
Materials, Getafe, Spain, Since July, 2016–May, 2017.

Visiting Faculty
Indian Statistical Institute, Kolkata, Jan.– Feb., 2016.

Senior Assistant Professor
VIT University, Vellore 632014, Tamil Nadu, India, June, 2015–Nov., 2015.

Academic Scientist-D (at the rank of Assistant Professor)
Thematic Unit of Excellence on Computational Materials Science (TUE-CMS), S. N. Bose National Centre for Basic Sciences, Sector-III, Salt Lake, Kolkata-70098, India, 2013–2015.

Postdoctoral Research Scholar
Dept. of Chemical Engineering, The Pennsylvania State University, PA. 2011–2012 Coarse-Grain molecular modeling to probe self assembly and membrane protein insertion in diblock-copolymer for bio-engineering applications.

Postdoctoral Research Associate
Center for Advanced Vehicular Systems, Mississippi State University, MS. 2010–2011

DFT-continuum linkage for Mg alloy, evolution of defects and deformation mechanism in nanocrys-talline metals to understand plastic and damage behavior.

Research Fellow

The Ames Laboratory, DOE Lab, Iowa State University, IA. May 1, 2009-July 31, 2009 Stress mapping in plastic deformation for Bulk Metallic Glass.

Research Assistant

Department of Physics and Astronomy, Mississippi State University, MS. 2006–2010 Physics of defects, multiscale modeling, interatomic potential development.

Research Assistant

Institute for Clean Energy Technology, Mississippi State University, MS. 2005–2006

Sensor development based on Raman Spectroscopy to determine the adulteration of Jet-fuel.

Scientific Assistant

Institute for Plasma Research (IPR), Dpt. of Atomic Energy, India. 2001–2005

Design and development of data acquisition system for quench detection and protection system for superconducting magnets; electrical, mechanical and hydraulic testing of magnetic coils.

Primary Teaching Areas

Solid State, Materials Science, Physical Metallurgy, Quantum and Classical mechanics, Thermody-namics, Statistical Physics, EM Theory, Lab-Based introductory Physics courses.

Courses Prepared/Taught*

- Multiscale Materials Modeling (ICME 4990/6990) with Mark F. Horstemeyer (30): Department of Mechanical Engineering, Mississippi State University, USA
- Laboratory Based Physics Course for UG (15): Department of Physics and Astronomy, Mississippi State University, USA
- Quantum Mechanics † (130): VIT-University, Vellore, India
- EM Theory † (130): VIT-University, Vellore, India
- Engineering Physics † (130): VIT University, Vellore, India
- Lab-Based introductory Physics courses † (120): VIT-University, Vellore, India

* The numbers in the parenthesis show the number of participants in each courses.

† Student Rating: 83–86 @VIT-University.

Primary Research Areas

Novel materials design & characterization with **ab initio** Density Functional Theory, molecular dy-namics and develop semi-empirical models, coarse-grain molecular modeling and phase-field simula-tions.

Computational Expertise

Linux, Python, C++, VASP, LAMMPS, OpenPhase

Awards and Achievements

- **Marie Curie Amarout-II Fellowship**, 2016
- A theory named after me: **Moitra's Order of Formability** http://journals.iop.org/cws/article/jpcm/58851
- **Editorial News Article in Journal of Technology**, 912, ISSN: 1944-1886, 2014
- **Fundamental Research Award for Light Metals**, TMS, 2011.
- **Sigma Xi** Outstanding graduate (PhD.) student award, 2010 and inducted to full membership.
- Awarded Travel Grant from SESAPS, 2009.
- Awarded a Travel Grant from MCC-UIUC, 2008.
- Awarded Masters in Physics with **summa cum laude** (GPA 4.0), 2007.
- 2nd Topper, Master of Science in Jadavpur University, 2002.
- Gold medalist in Bachelor of Science from University of Calcutta, 1999.
- National scholarship holder for undergraduate study, 1996.

Professional Affiliations

- Lifetime member of Plasma Science Society of India
- Member of American Physical Society
- Member of Sigma Xi
- Member of The Metals, Minerals, Materials Society (TMS)

Advisees

Undergraduates:

- Shashank Harivyasi, Summer, 2013
- Suman Kandal, Summer, 2011
- Marthony Robbins, Summer, 2011

Development of CyberInfrastructure.

- Michael Kim (Vanderbilt University) Summer, 2010

CyberInfrastructure: Graphical Molecular Editor (Edmol).

- Shashwat Namdeo, Summer, 2010
- Seongwon Hwang (Pohang Univ. of Sc. & Tech., Korea) Summer, 2010

Deformation mechanisms of Ni nano-pillar, and nano-wire.

- Shashank Harivyasi on "Vacancy effect on nanowire deformation mechanism."

Co-Advisor, PhD Students:

- Mehul Bhatia* on "Atomistic simulations for computational materials design."
- Ilaksh Adlakha* on "Impurity effect on nanoscale materials deformation."
- Poulami Chakraborty on "Hydrogen interactions with defects in bulk Zr."

* Discontinued guiding after I left USA

Services

Facility Establishment: CRAY XE6 with 7808 cores 2.6GHz with 75 TF peak having 3D Torus Interconnect, commissioned with required Precision Air-Conditioner, Uninterrupted Power Supply and data-centre preparation involving both false ceiling and floor. (110 million INR)

Online Teaching: Methodology for electronic scale simulation in Cyber Infrastructure. https://ccg.hpc.msstate.edu/mediawiki/index.php/MaterialModels

Journal Reviewing: Phys. Rev. B, Computational Materials Science, Materials Science & Engineering B., Materials Letters.

Submitted and Funded Research Proposals

9. "Computational Design of Al-Mg Alloys", 200,000 Euro, Regional Govt. of Madrid, (**Pend-ing**.)
8. "Technology Research Centre at S. N. Bose National Centre for Basic Sciences", 110,00,00,000 INR, DST, (**Funded, 2015*** .)
7. "Development and Validation of a Modified Embedded Atom Method (MEAM) Potential for Aluminum Alloys", 25,00,000 INR, DAE-BRNS, (**Funded 22,00,000**.)
6. "Computational design of Mg-Li alloys: A hierarchical multiscale method", $5000, June, 2014– June, 2015, DST-DAAD proposal (**Prepared with Sebastien Groh, Freidburg, Ger-many**)
5. "Analysis of Environmental Effects on the Crack Tip Stress Field using an Atomistic-Dislocation Approach", $536 K, Aug., 2011–Aug., 2015, ONR Basic Science Program, (**Funded in col-laboration with Prof. K. N. Solanki at ASU**.)

4. "Coarse Grain Model of Anticancer Drug Delivery Systems", $500 K, Aug.2012–July, 2017, Burroughs Wellcome Fund CASI (**Not funded**).

3. "A method to increase the additional slip systems to enhance the formability of polycrystalline Magnesium alloys", $231 K, Feb., 2012, NSF (**Prepared for NSF**.)
2. "Integrated Multi-scale Modeling for Accelerated Aging of Used Nuclear Fuel in Storage", $1.5 M, June, 2011-June, 2013, INL (**Funded*** .)
1. "Applicability of Atomic Simulation to Hydrogen Assisted Cracking", $160 K, Feb., 09-Sep 11, ONR Basic Science Program. (**Funded*** .)

* Contributed substantially to idea and collaboration development and writing for these proposals.

Publications (50)
Book Chapters (4)

4. K. N. Solanki, **A. Moitra** and M. Bhatia "Effect of Substituted Aluminum in Magnesium Tension Twin" **Essential Readings in Magnesium Technology 2014, Eds. Suveen N. Math-audhu, Alan A. Luo, Neale R. Neelameggham, Eric A. Nyberg, W. H. Sillekens, John Wiley and Sons, Inc., Hoboken, NJ, USA; Pages:479–483; ISBN:9781118858943**.

3. Mark Horstemeyer, **Amitava Moitra** "Electronic scale simulations for the multiscale mod-eling" **Integrated Computational Materials Engineering for Metals: Using Multiscale Modeling to Invigorate Engineering Design with Science, July, 2012, John Willey & Sons Inc., ISBN: 9781118022528**.

2. K. Solanki, **Amitava Moitra** and M. Bhatia "Effect of Substituted Aluminum in Magnesium Tension Twin" **Magnesium Technology 2011, Eds. Wim H. Sillekens, Sean R. Agnew, Ne ale R. Neelameggham, Suveen N. Mathaudhu, John Wiley and Sons Ltd. April 2011, Pages:668; ISBN:9781118029367**.

1. **Amitava Moitra**, Sungho Kim, Seong-Gon Kim, Seong Jin Park, Randall German, and Mark Horstemeyer "Atomistic scale study on effect of crystalline misalignment on densification during sintering nano scale tungsten powder," **Advances in Sintering Science and Technology, eds. Rajendra K. Bordia and Eugene A. Olevsky, pg. 149-160 ISBN:9780470408490, Feb., 2010**.

Peer Reviewed Journals
Published (25)

25. Suvankar Das, **Amitava Moitra**, Mishreyee Bhattacharya, Amlan Dutta, "Thermal stress and buckling instability in Si/Ge and Ge/Si core/shell nanowires" **Beilstein J. Nanotechnol., 6, 1970, 2015**.

24. Vivek Dixit, Chandani Nandadasa, Sungho Kim, Jihoon Park, **Amitava Moitra**, Laalitha Liyanage, Yang-Ki Hong, Seong-Gon Kim "Site occupancy and magnetic properties of Al-substituted M-type strontium hexaferrite". **J. App. Phys., 117, 243904, 2015**.

23. Poulami Chakravorty, **Amitava Moitra**, Tanusri Saha-Dasgupta "Effect of hydrogen on degradation mechanism of Zirconium: A Molecular Dynamics study". **J. Nuclear Materi-als, 466, 172–178, 2015** (IF:1.865).

22. Amlan Dutta, Swastika Bhattacharya, Arup K. Raychaudhuri, **Amitava Moitra**, Tanusri Saha-Dasgupta "In-silico investigation of Rayleigh instability in ultrathin copper nanowire in premelting regime". **J. App. Phys, 115, 244303, 2014** (IF:2.528).

21. **Amitava Moitra**, Seong-Gon Kim, M. F. Horstemeyer "Solute effect on hC + Ai dislocation nucleation mechanism on magnesium". **Acta Materialia, 75, 106-112, 2014** (IF:4.395). ******
Editorial News Article in Journal of Technology, 912, ISSN: 1944-1886, Pubz ID: 009215695

20. **Amitava Moitra**, Seong-Gon Kim, M.F. Horstemeyer "Solute effect on basal and prismatic slip systems in Mg" **J. Phys.: Condens. Matter, 26 (44), 445004, 2014** (IF:2.355).

19. **Amitava Moitra**, Sungho Kim, Seong-Gon Kim, S. C. Erwin, Yang-Ki Hong, Jihoon Park "Site occupancy and magnetic properties of aluminum substituted M-type barium hexaferrite "**Computational Condensed Matter, 1, 45–50, 2014** (IF:1.826).

18. Ebrahim Asadi, Mohsen Asle Zaeem, **Amitava Moitra**, Mark Tschopp "Vacancy effect on Generalized Stacking Fault Energy for FCC and HCP metals" **J. Phys.: Condens. Matter, 26, 115404, 2014: IOP Editor's Choice** (IF:2.355).

17. **Amitava Moitra** "Grain size effect on microstructural properties of 3D nanocrystalline mag-nesium under tensile deformation" **Comp. Mater. Sc., 79, 247–251 2013** (IF:1.965).

16. Mehul Bhatia, **Amitava Moitra**, Kiran N. Solanki, Mark A. Tschopp "Investigating Dam-age Evolution at the Nanoscale: Molecular Dynamics Simulations of Nanovoid Growth in Single-Crystal Aluminum" **Metallurgical and Materials Transactions A, 44, 2, 617–626 2013** (IF:1.627).

15. Bohumir Jelinek, S. Groh, M.F. Horstemeyer, J. Houze, S. G. Kim, G. J. Wagner, **Amitava Moitra**, M. I. Baskes "Modified Embedded Atom Method potential fo Al, Si, Mg, Cu, and Fe alloys"**Phys. Rev. B: 85, 245102–245120 2012** (IF:3.767).

14. **Amitava Moitra**, Seong-Gon Kim, M. F. Horstemeyer "Structural and thermal properties of Calcium with a MEAM potential "**CALPHAD, 35, 2, 262–268 2011** (IF:1.775).

13. **Amitava Moitra**, Kiran N. Solanki "Adsorption and penetration of hydrogen in W: A first principles study" **Comp. Mater. Sc., 50, 7, 2291–2294, 2011** (IF:1.965).

12. **Amitava Moitra**, Seong-Gon Kim, Seong J. Park, M. F. Horstemeyer "The effect of Vanadium-Carbide monolayer on Tungsten and Carbon adsorption on Tungsten Carbide"**Science of Sin-tering, 43, 153–159, 2011** (IF:0.403).

11. **Amitava Moitra**, Kiran N. Solanki, M.F. Horstemeyer "The location of atomic hydrogen in NiTi alloy: a first principles study" **Comp. Mater. Sc., 50, 3, 820-823, 2011** (IF:1.965).

10. **Amitava Moitra**, S. Kim, S-G. Kim, S.J. Park, R. M. German, M. F. Horstemeyer "Atom-istic scale study on effect of crystalline misalignment on densification during sintering nano scale tungsten powder"**Ceramic Transactions, Vol 209, pg: 149–160, 2010** (IF:0.447).

9. **Amitava Moitra**, Sungho Kim, Seong-Gon Kim, Seong Jin Park, R. M. German, and M.F. Horstemeyer "Investigation on sintering mechanism based on atomistic simulations" **AIP Con-ference Series, Vol 1252, pg. 1176–1183, 2010** (IF:2.093).

8. J. Jalli, Y. K. Hong, S. Bae, J. J. Lee, G. S. Abo, J. H. Park, **A. Moitra**, S. Kim, S. C. Erwin, M. J. Kim & T. Tanaka "Conversion of Worm-Shaped Antiferromagnetic Hematite to Ferrimagnetic Spherical Barium-Ferrite Nanoparticles for Particulate Recording Media" **IEEE Magn. Lett., Vol. 1, pg. 4500204, 2010** (IF:1.48).

7. S. J. Park, S. Ahn, T. G. Kang, S. T. Chung, Y. S. Kwon, S. H. Chung, S. Kim, **A. Moitra**, & R. M. German "A Review of Computer Simulations in Powder Injection Molding" **Inter. Jrnl. Powder Metallurgy, Vol. 46, No. 3, pg. 37–46, 2010** (IF:0.584).

6. **Amitava Moitra**, Sungho Kim, Seong-Gon Kim, Seong Jin Park, Randall M. German, M. F. Horstemeyer "Investigation on sintering mechanism of nanoscale Tungsten powder based on atomistic simulation "**Acta Materialia, 58, 11, 3939, 2010** (IF:4.395).

5. Kim, Seong-Gon, Horstemeyer, M. F., Baskes, M.I., Rais-Rohani, M., Kim, Sungho, Jelinek, B., Houze, J., **Amitava Moitra**, and Laalitha L. "Semiempirical potential methods for atom-istic simulations of metals and their construction procedures" **Journal of Engineering Materials and Technology,Vol. 131, Issue 4, 041210 (9pp) Oct. 2009** (IF:1.89).

4. Jalli, Jeevan; Hong, Yang-Ki; Bae, Seok, Abo, Gavin, Lee, Jae-Jin, Sur, Jung-Chul, Gee, Sung-Hoon, Kim, Seong-Gon, Erwin, Steven, **Amitava Moitra** "Conversion of Nano-sized Spherical Magnetite to Spherical Barium Ferrite Nanoparticles for High Density Particulate Recording Media" **IEEE Transactions on Magnetics, Vol 45, No. 10, 3590 (4pp), Oct. 2009** (IF:1.422).

3. **Amitava Moitra**, Sungho Kim, Jeff Houze, Bohumir Jelinek, Seong-Gon Kim, Seong-Jin Park, Randall M German, Mark F Horstemeyer "Melting Tungsten nanoparticles: a molecular dynamic study" **J. Phys. D: Appl. Phys. 41, 185406 (7pp) (2008), August, 2008** (IF:2.528).

2. Vidhu S. Tiwari, **Amitava Moitra**, Rajamohan R. Kalluru, Fang-Yu Yueh, Jagdish P. Singh "Laser raman optical sensor for monitoring gas mixtures using photomultiplier tube detector" **Progress in Biomedical Optics and Imaging, Vol 6377, 63770, 2006** (IF:0.982).

1. A. N. Sharma, C. J. Hansalia, Y. Yeole, G. Bansal, S. Pradhan, **Amitava Moitra**, Y. C. Saxena "Quench detection and data acquisition system for SST-1 superconducting magnets," **Fusion Engineering and Design, Vol. 74, Issues 1-4, pg. 819-823 2005**, (IF:0.942).

In preparation (6)

6. **Amitava Moitra**, Javier Llorca "Atomistic based Precipitation Hardening Mechanism on Mg-Al alloy in athermal limit". **preparing for Jrnl. Mechanics and Physics of Solids**.

5. Gustavo Esteban Manzanares, **Amitava Moitra**, Javier Llorca, Javier Segurado "Solid solu-tion strengthening of Mg alloys". **preparing for Acta Materialia**.

4. **Amitava Moitra**, Javier Llorca "Twin engulfed Precipitate in AZ-91: An MD Study". **preparing for Materials Letters**.

3. **Amitava Moitra**, Amlan Dutta, Sajeev Chacko, "Computational study of Cu-Ni core-shell nanoparticles". **Jrnl. of Physics D: Applied Physics**.

2. Mishreyee Bhattacharya, **Amitava Moitra**, Amlan Dutta, "Characterizing deformation for Cu-Zr bulk metallic glass". **preparing for Phys. Rev. B**.

1. **Amitava Moitra**, Amlan Dutta and Seong-Gon Kim "Mechanical and thermal properties of Fe with V impurities using a MEAM interatomic potential". **preparing for Phys. Rev. B**.

Peer Reviewed Conference Papers (17)

17. Ebrahim Asadi, Mohsen Asle Zaeem, **Amitava Moitra**, Mark Tschopp "Vacancy effect on Generalized Stacking Fault Energy for FCC and HCP metals" **TMS 2014 Proceedings, San Diego, California**.

16. Mehul Bhatia, Kiran N. Solanki, **Amitava Moitra**, Mark Tschopp "Nanoscale Investigation of Twinning and Detwinning during Starin-Path Changes in Magnesium"**TMS 2012 Proceed-ings, Orlando, FL**.

15. Ilaksh Adlakha, Kiran N. Solanki, **Amitava Moitra**, Mark Tschopp "A Nanoscale Investiga-tion on Effect of Hydrogen in Confined Volumes"**TMS 2012 Proceedings, Orlando, FL**.

14. Ilaksh Adlakha, Kiran N. Solanki, **Amitava Moitra**, Mark Tschopp "Influence of Size on Strength of Nickel Nanowires"**TMS 2012 Proceedings, Orlando, FL**.

13. Mehul Bhatia, Kiran N. Solanki, **Amitava Moitra**, Mark Tschopp "Role of Substituted El-ements on Twinning Nucleation Mechanism in Magnesium"**TMS 2012 Proceedings, Orlando, FL**.

12. Horstemeyer Mark, **Moitra Amitava**, Solanki, K.N., "Deformation of Polycrystalline Mag-nesium Thin Film Size Effects" **American Institute for Mechanical Engineers (AIME) TMS 2011 Proceedings, San Diego, CA**.

11. **Amitava Moitra**, Solanki, K.N. "Effect of Substituted Aluminum in Magnesium Tension Twin"**TMS 2011 Proceedings, San Diego, CA**.

10. **Amitava Moitra**, Solanki, K.N., Horstemeyer M. F. "Size Scale Effect on the Deformation of 3D Nanocrystalline Magnesium" **TMS 2011 Proceedings, San Diego, CA**.

9. **Amitava Moitra**, Solanki, K.N., Tschopp M. A. "The Effect of Crystallographic Orientation on Void Growth: A Molecular Dynamics Study" **TMS 2011 Proceedings, San Diego, CA**.

8. Bhatia, M., **Amitava Moitra**, Solanki, K.N., Tschopp M. A., and Horstemeyer, MF "Defor-mation of Nanovoid in a Single Crystal Aluminum"**TMS MS&T 2010, Houston, TX** .

7. J. H. Park, Y. K. Hong, S. Bae, J. J. Lee, G. S. Abo, J. Jalli, J. C. Choi, J. G. Lee, S. G. Kim, and **A. Moitra**, "First-principles Calculations of Magnetic Moment and Anisotropy Constant for LTP MnBi",**Joint International Conference on the 7th Asian Meeting on Fer-roelectricity and the 7th Asian Meeting on Electroceramics, June 28-July 1, Jeju, South Korea.**

6. **Amitava Moitra**, Sungho Kim, Seong-Gon Kim, Seong Jin Park, R. M. German, and MF Horstemeyer "Investigation on sintering mechanism of nanoscale tungsten powder based on atomistic simulations" **AIP Conference Proceedings: 10TH International Conference on Nu-merical Methods in Industrial Forming Processes (Vol. 1252, pp. 1176–1183, June 2010)**.

5. **Amitava Moitra**, Sungho Kim, Seong-Gon Kim, Seong Jin Park, R. M. German "Atomistic scale study on sintering of nano scale Tungsten powder" **ACerS International Conference on Sintering 2009 proceedings**.

4. **Amitava Moitra**, Sungho Kim, Seong-Gon Kim, Seong Jin Park, R. M. German "Three di-mensional atomistic simulation of the sintering and shrinkage behavior of nanoscale Tungsten." **Proceedings of the International Conference on Tungsten, Refractory and Hardmaterials VII, Metal Powder Industries Federation, Princeton, NJ. June, 2008**.

3. **Amitava Moitra**, Sungho kim, Seong-Gon Kim, Seong Jin Park, Randall M. German "Atom-istic simulation of activation sintering mechanism of Tungsten by additives." **Advances in Powder Metallurgy and Particulate Materials 2007, Denver, CO, 1, 70-75. July, 2007**.

2. Vidhu S. Tiwari, **Amitava Moitra**, R. Kalluru, Fang-Yu Yueh, J. P. Singh "Laser Raman optical sensor for monitoring gas mixtures using photomultiplier tube detector" **Proceedings SPIE, vol 6377, 63770L (2006), Boston, MA, USA, Oct, 17, 2006**.

1. G. Bansal, S. Pradhan, B. Sarkar, A. N. Sharma, V. Rathod, U. Prasad, **Amitava Moitra**, R. Behl, K.J. Thomas, B.R. Doshi, P. Chauhan, Y. C. Saxena "Joints fabrication in supercon-ducting magnets of SST-1" **Proceedings, Symposium on Fusion Engineering, 2003, pg. 589-592**.

Professional Presentations (10)

10. **Amitava Moitra** "Evolution of defects and their interactions: An MD study" **Phy. & Chem of Mater: Comput. & Expt. 2014, Kolkata, India, Invited Talk, Feb. 24-25, 2014**.

9. **Amitava Moitra** "Linking DFT results to continuum scale model in determining alloying effects in mechanical properties of Mg alloys" **IUMRS-ICA 2013, Bangalore, India, Dec. 16-20, 2013**.

8. Kiran N. Solanki, **Amitava Moitra**, Mehul Bhatia "Effect of Substituted Aluminum in Mag-nesium Tension Twin" **The minerals, metals and materials society (TMS), San Diego, CA, 2011**.

7. M. F. Horstemeyer, **Amitava Moitra**, Kiran N. Solanki "Deformation of Polycrystalline Mag-nesium Thin Film Size Effects" **TMS, San Diego, CA, 2011**.

6. Kiran N. Solanki, **Amitava Moitra**, Mehul Bhatia, Mark Tschopp "Deformation, Damage, and Fracture of Light Metals and Alloys" **The minerals, metals and materials society (TMS), San Diego, CA, 2011**.

5. **Amitava Moitra**, Mehul Bhatia, Kiran N. Solanki "Orientation effect on dislocation nucle-ation and related interaction during void growth simulations in Aluminum" **American Physical Society (APS), Dallas, TX, 2011**.

4. **Amitava Moitra**, Sungho Kim, Seong-Gon Kim, Yank-Ki Hong, Steven Erwin "Site oc-cupancy and magnetic properties Aluminum substituted Barium hexaferrite" **South Eastern Section of American Physical Society (SESAPS), Atlanta, GA, Nov. 11-14, 2009**.

3. **Amitava Moitra**, Sungho Kim, Bohumir Jelinek, Jeff Houze, Seong-Gon Kim "EAM inter-atomic potential for Zinc" **APS March Meeting, New Orleans, LA, USA, March 10-14, 2008**.

2. **Amitava Moitra**, Sungho kim, Seong-Gon Kim, Seong Jin Park, Randall M. German "Molec-ular dynamics simulation of sintering of Tungsten nanopowders" **Mississippi Academy of Sci-ence, Starkville, MS 2007**.

1. **Amitava Moitra**, Sungho Kim, Seong-Gon Kim "Molecular dynamics simulation of sintering of nanopowders" **South Eastern Section of American Physical Society, Williamsburg, VA Nov 9-11, 2006**.

Poster Presentations (02)

2. T. Saha-Dasgupta, R. Biswas, P. Mahadevan, J. Chakraborty, S. Chatterjee, P. Pradhan, M. Kumar, A. Moitra, B. Mukherjee, S. Chako"Computational study on soft and hard materials" **Nano-Mission, Bangalore, India, 2013**.

1. Kiran N. Solanki, **Amitava Moitra** "Effect of H in Metals and Alloys: An Application to bcc W and NiTi Alloy" **The minerals, metals and materials society (TMS), San Diego, CA, 2011**.

Contributed Presentations (12)

12. Ebrahim Asadi, Mohsen Asle Zaeem, **Amitava Moitra**, Mark Tschopp "Vacancy effect on Generalized Stacking Fault Energy for FCC and HCP metals" **TMS 2014, San Diego, Califor-nia**.

11. Kiran Solanki, **Amitava Moitra**, Mehul Bhatia "Dislocation interaction during void growth simulation" **US National Congress on Computational Mechanics, Minnesota, July 25-28, 2011**.

10. M. I. Baskes, B. Jelinek, S. Groh,**Amitava Moitra**, M. F. Horstemeyer, J. Houze, S. G. Kim, G. J. Wagner "New MEAM Potentials for the Al, Si, Mg, Cu, and Fe Alloy System" **NIST Atomistic Simulations for Industrial Needs, Gaithersburg, MD, June 23-24, 2011**.

9. Seong-Gon Kim, **Amitava Moitra**, Sungho Kim, Seong Jin Park, Randall German "Atomistic simulations of nanoparticle sintering" **International Conference on Powder Injection Molding & Workshop on Medical Applications of Micro PIM, Orlando, FL, March 2-5, 2009**.

8. **Amitava Moitra**, Sungho Kim, Seong-Gon Kim, Seong Jin Park, Randall German, Mark Horstemeyer "Atomistic scale study on effect of crystalline misalignment on densification dur-ing sintering nano scale Tunsten powder" **International Conference on Sintering 2008, Cali-fornia, Nov 16-20, 2008**.

7. Bohumir Jelinek, **Amitava Moitra**, Seong-Gon Kim "Development of EAM potential for Fe-C alloys system" **APS March Meeting, New Orleans, LA, March 10-14, 2008**.

6. **Amitava Moitra**, Sungho Kim, Seong-Gon Kim, Seong Jin Park, Randall German, Mark Horstemeyer "Atomistic scale study on effect of pressure on densification during sintering nano scale Tungsten powder" **TMS 2008 Annual Meeting, New Orleans, LA, March 11, 2008**.

5. **Amitava Moitra**, Sungho Kim, Seong Jin Park, Randall German, Seong-Gon Kim "Linkage between atomistic and continuum based simulations in nanoscale powder metallurgy" **Ad-vanced computational materials science and engineering methods, Orlando, FL, Feb 27, 2007**.

4. **Amitava Moitra**, Randall German, Seong-Gon Kim "Atomistic simulation for activation sin-tering mechanism of Tungsten by additives" **The Powder Met., Denver, CO, May 13- 17, 2007**.

3. **Amitava Moitra**, Sungho Kim, Seong Jin Park, Randall German, Seong-Gon Kim "Atomistic simulation of activated sintering of Tungsten by additives" **Metal Powder Industries Federa-tion, Technical Session, Jan, 2007**.

2. Sungho Kim, **Amitava Moitra**, Seong-Gon Kim, Mark Horstemeyer "First principles study of FCC-HCP interface dynamics under uniaxial tension" **South Eastern section of American Physical Society, Williamsburg, VA, Nov 9-11, 2006**.

1. V. Tiwari, **Amitava Moitra**, R. Kalluru, J. P. Singh "Determination of concentration ratio of nitrogen and oxygen in a liquid mixture" **Optics East conference held at MIT, MA, Oct., 2006**.

Workshops/Symposia Attended

4. **LAMMPS Users' Workshop; Sponsored by Sandia National Laboratories Albu-querque, New Mexico, USA, Aug. 9–11, 2011**.
3. **NIST Workshop on Atomistic Simulations for Industrial Needs Gaithersburg, MD, June 23–24, 2011**.
2. **Symposium on Predictive Science and Technology in Mechanics and Materials Starkville, June 22–25, 2010 & June 23–25, 2008**.
1. **Electronic Structure Workshop 2008 20th Annual Workshop on Recent Developments in Electronic Structure Methods, University of Illinois at Urbana-Champaign 2008, June 18–20, 2008**.

Workshops/Conference Organized

Physics and Chemistry of Materials: Computation and Experiments S.N. Bose Centre, Kolkata, Feb 24-25, 2014.

Professional International Invitations (5)

5. 2012 International Conference on Geology of Mineral Deposits **Ulan-Ude, Russia, March 20– 24 2012**
4. International Conference on Drug Discovery and Therapy **Dubai, UAE, Feb 12–15, 2012**
3. International Conference on Environmental Security for Food and Health **Cape Comarin, Tamil Nadu, India, Feb 16–18, 2012**
2. Progress in Nanoscience and Materials **Sanghai, China, Dec. 20–22, 2011**
1. Montreal International Translational Medicine Conference **Montreal, Quebec, Canada, Nov 3– 4, 2011**

Invited Talk (8)

8. **Jawaharlal Nehru Centre for Advanced Scientific Research**, "Multiscale Materials Modeling" 2012
7. **Harish Chandra Research Institute**, "Magnesium Alloy Design: A perspective on multi-scale modeling" 2012
6. **National Physical Laboratory**, "Computational Materials Modeling for Mg alloys" 2012
5. **Institute for Plasma Research**, "Computational Alloy Design for Mg Alloys" 2012
4. **CSIR Fourth Paradigm Institute, (Formerly CMMACS)**, "Mg Alloy Design using computational approaches" 2012
3. **National Physical Laboratory, New Delhi**, "An Overview of Muliscale Materials Model-ing" 2012
2. **Indian Institute of Technology-Ropar**, "Mg Alloy Design: A perspective on multiscale materials modeling" 2012
1. **Indian Institute of Technology-Hyderabad**, "Integrated Computational Materials Engi-neering to design novel Alloys", 2014