

# SOUMIK BANERJEE, Ph.D.

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## CONTACT

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## PROFESSIONAL PREPARATION

**PhD**, Engineering Mechanics, Virginia Tech, Blacksburg, 2008.

**MS**, Mechanical Engineering, University of Illinois at Chicago, 2004.

**BME**, Mechanical Engineering, Jadavpur University, Kolkata, India, 2002.

## APPOINTMENTS

- 08/17-present Associate Professor, School of Mechanical and Materials Engineering,  
Washington State University (WSU)
- 08/13-present Member Faculty, Materials Science and Engineering Program, WSU
- 08/11-07/17 Assistant Professor, School of Mechanical and Materials Engineering, WSU
- 11/09-07/11 Postdoctoral Research Fellow, Mechanical Engineering Department, University  
of Michigan – Ann Arbor
- 08/08-10/09 Postdoctoral Research Scholar, Max Planck Institute for Dynamics of Complex  
Technical Systems, Germany
- 08/04-07/08 Research & Teaching Assistant, Engineering Science and Mechanics, Virginia  
Tech
- 08/02-07/04 Research Assistant, Mechanical Engineering, University of Illinois at Chicago

## RESEARCH INTERESTS

Molecular modeling of self-assembly, chemical kinetics and transport phenomena in materials and interfaces relevant to energy conversion and storage devices

- Morphology of photoactive layers and electron transport layers in photovoltaic solar cells
- Anode-glassy electrolyte interfaces in all solid state sodium ion batteries
- Lithium ion transport through ionic liquid electrolytes in batteries
- Multiscale modeling of agglomeration and growth of nanostructures
- Grain boundary diffusion in tin and tin-indium and tin-lead alloys

## AWARDS AND HONORS

- Received the **3M Non-tenured Faculty Award**, 2013 – 2016
- **Certificate of appreciation** for “valued services in advancing the engineering profession as session and track organizer” at the ASME 2016 Power and Energy Conference
- Received the **GPSA Academic Advisor Excellence Award** at WSU, 2014
- National Science Foundation (NSF) Fellowship to attend the Summer Institute on “**Materials Genome**”, Northwestern University, 2013
- Selected in *Cambridge Who’s Who Executives, Professionals and Entrepreneurs*, 2010
- Visiting scientist at **FOM Institute**, Netherlands, December 2008
- **Max Planck Research Stipendium**, August 2008

- National Science Foundation (NSF) Fellowship to attend the Summer Institute on “**Energy Challenge and Nanotechnology**”, Northwestern University, 2008
- **Dean’s Pratt Fellowship** from Virginia Tech for research and academic accomplishments, Spring 2007 and Fall 2006
- **Best poster award** from the **Dean’s Forum on Energy Security and Sustainability** at Virginia Tech for the presentation titled “Synthesis of Carbon Nanotubes and their Hydrogen Storage Capacity”, Fall 2006

#### INVITED TALKS

- Invited talk at *Theory and Applications of Computational Chemistry* Conference, 2016
- Invited talk at Pacific Northwest National Lab, 2016
- Invited talk at NSF-IUSSTF Indo-US Workshop on Analysis of Multiphysics Phenomena in Li-ion Cells held in Indian Institute of Technology, Bombay, 2016
- Invited talk at Jadavpur University, India, 2016
- Invited talk at Physics Colloquium, University of Idaho, October 2015
- Invited talk at The Boeing Company, September, 2013
- Invited talk at Math Colloquium, University of Idaho, March 2013
- Invited talk at Dow Chemical Company, Freeport, Texas, November 2012
- Invited talk at Texas Tech University, Lubbock, Texas, March 2011
- Invited talk at DOE Office of Science Graduate Fellowship (DOE SCGF) Research Meeting, Argonne National Lab, August 2010

#### PUBLICATIONS IN PEER REVIEWED JOURNALS AND CONFERENCE PROCEEDINGS

1. K. Yoo, S. Banerjee, J. Kim, and P. Dutta, “A review of modeling studies for Li-air battery”, *Energies*, vol. 10, 1748, 2017
2. A. Dive, and S. Banerjee, “Ion storage in nano-confined interstices between vertically aligned nanotubes in electric double-layer capacitors”, *Journal of Electrochemical Energy Conversion and Storage*, 15(1), 011001, Emerging Investigators in Electrochemical Energy Conversion and Storage 2017
3. K. Shah, N. Balsara, S. Banerjee, M. Chintapalli, W. Chiu, A. Cocco, I. Lahiri, S. Martha, A. Mistry, P. Mukherjee, V. Ramadesigan, C. Sharma, V. Subramanian, S. Mitra, and A. Jain, “State-of-the-art and future research needs for multiscale analysis of Li-ion cells”, *Journal of Electrochemical Energy Conversion and Storage*, vol. 14, 020801-17, 2017
4. SM Mortuza, and S. Banerjee, “Atomistic modeling – Impact and opportunities in thin-film photovoltaic solar cell technologies”, *Molecular Simulation*, vol. 43 (10-11), pp. 774 – 796, 2017
5. A. Dive, M.K. Song, and S. Banerjee, “Physisorption of solvated polysulfide chains on graphene oxides with varied topologies and functional groups”, *Journal of Physical Chemistry C*, vol. 121 (9), pp. 5089–5098, 2017
6. SM Mortuza, MFN Taufique, and S. Banerjee, “Solution processed deposition of electron transport layers on perovskite crystal surface – A modeling based study”, *Applied Surface Science*, vol. 394, pp. 488-497, 2017
7. MFN Taufique, SM Mortuza, and S. Banerjee, “A mechanistic insight into attachment of fullerene derivatives on crystal faces of methyl ammonium lead iodide based

- perovskites”, *Journal of Physical Chemistry C*, vol. 120, pp. 22426–22432, 2016
8. S. Kazemiabnavi, Z. Zhang, K. Thornton, and S. Banerjee, “Electrochemical stability window of ionic liquids as the electrolytes for lithium batteries”, *Journal of Physical Chemistry B*, vol. 120, pp. 5691–5702, 2016
  9. S. Banerjee, I. Dutta, and B.S. Majumdar, “A molecular dynamics evaluation of the effect of dopant addition on grain boundary diffusion in tin: Implication for whisker growth”, *Materials Science & Engineering A*, vol. 666, pp. 191–198, 2016
  10. K. Yoo, A. Dive, S. Kazemiabnavi, S. Banerjee, and P. Dutta, “Effects of operating temperature on the electric performance of a Li-air battery operated with ionic liquid electrolyte”, *Electrochimica Acta*, vol. 194, pp. 317–329, 2016
  11. A. Dive, and S. Banerjee, “Graphene/Sulfur and Graphene oxide (GO)/Sulfur composite cathodes for high performance Li-S batteries: A molecular dynamics study”, *Proceedings of IMECE 2016*, ASME IMECE, Phoenix, 2016
  12. K. Yoo, A. Deshpande, S. Banerjee and P. Dutta, “Electrochemical model for ionic liquid electrolytes in lithium batteries”, *Electrochimica Acta*, vol. 176, pp. 301-310, 2015
  13. S.M. Mortuza, L.K. Kariyawasam and S. Banerjee, “Combined deterministic-stochastic framework for modeling the agglomeration of colloidal particles”, *Physical Review E*, vol. 92, 013304, 2015
  14. S. Kazemiabnavi, P. Dutta, and S. Banerjee, “A density functional theory based study of the electron transfer reaction at the cathode-electrolyte interface in lithium-air battery”, *Physical Chemistry Chemical Physics*, vol. 17, pp. 11740 - 11751, 2015
  15. K. Yoo, S. Banerjee, and P. Dutta, “Electrochemical Model for Ionic Liquid Electrolytes in Lithium Batteries”, *Proceedings of IMECE 2015*, ASME IMECE, Houston, 2015
  16. L.M. Meinshausen, S. Banerjee, I. Dutta, B. Majumdar, “Mitigation of tin whisker growth by dopant addition”, *Proceedings of ASME InterPACK/ICNMM 2015*, San Francisco.
  17. S. Banerjee, “A group project based approach to induce learning in engineering thermodynamics”, *Proceedings of the ASEE’s 122<sup>nd</sup> Annual Conference and Exposition*, Seattle, 2015
  18. S. Kazemiabnavi, P. Dutta, and S. Banerjee, “Density functional theory based study of the electron transfer reaction at the lithium metal anode in lithium-air battery with ionic liquid electrolytes”, *Journal of Physical Chemistry C*, vol. 118, pp. 27183–27192, 2014
  19. M. Mostafa, and S. Banerjee, “Predictive model for alignment and deposition of functionalized nanotubes using applied electric field”, *Journal of Applied Physics*, vol. 116, 244309, 2014
  20. M. Mostafa, and S. Banerjee, “Effect of functional group topology of carbon nanotubes on electrophoretic alignment and properties of deposited layer”, *Journal of Physical Chemistry C*, vol. 118, pp. 11417-11425, 2014
  21. K. Yoo, S. Banerjee and P. Dutta, “Modeling of Volume Change Phenomena in a Li-Air Battery”, *Journal of Power Sources*, vol. 258, pp. 340-350, 2014
  22. P.P.S. Saeed Abadi, M.R. Maschmann, S.M. Golam Mortuza, S. Banerjee, J.W. Baur, S. Graham, and B.A. Cola, “Reversible tailoring of mechanical properties of carbon nanotube forests by immersing in solvents”, *Carbon*, vol. 69, pp. 178–187, 2014
  23. A. Deshpande, P. Dutta, and S. Banerjee, “Solubility of oxygen in lithium-air battery

- electrolytes: a molecular dynamics study”, accepted, *Proceedings of IMECE 2014*, ASME IMECE, Montreal, 2014
24. K. Yoo, S. Banerjee, and P. Dutta, “A mathematical model for li-air battery considering volume change phenomena”, accepted, *Proceedings of IMECE 2014*, ASME IMECE, Montreal, 2014
  25. S. Kazemiabnavi, P. Dutta, and S. Banerjee, “Ab initio modeling of the electron transfer reaction rate at the electrode-electrolyte interface in lithium-air batteries”, accepted, *Proceedings of IMECE 2014*, ASME IMECE, Montreal, 2014
  26. A. Deshpande, L. Kariyawasam, P. Dutta, and S. Banerjee, “Enhancement of lithium ion mobility in ionic liquid electrolytes in presence of additives”, *Journal of Physical Chemistry C*, vol. 117, pp. 25343–25351, 2013
  27. S.M. Mortuza, C. Cisneros, M. Bartolo, and S. Banerjee, “Molecular modeling of nanoparticles and conjugated polymers during synthesis of photoactive layers of organic photovoltaic solar cells”, *Proceedings of AIChE Annual Meeting*, San Francisco, 2013
  28. S.M. Mortuza, and S. Banerjee, “Controlled self-assembly of functionalized carbon nanotubes on silicon substrates”, *Proceedings of IMECE 2013*, ASME IMECE, San Diego, 2013
  29. S.M. Mortuza, and S. Banerjee, “Solvent-based preferential deposition of functionalized carbon nanotubes on substrates”, *Journal of Applied Physics*, vol. 114, 074301, 2013
  30. S. Banerjee, “Molecular dynamics study of self-agglomeration of charged fullerenes in solvents”, *Journal of Chemical Physics*, vol. 138, 044318, 2013
  31. S.M. Mortuza, and S. Banerjee, “Molecular modeling study of agglomeration of [6,6]-phenyl-C61-butyric acid methyl ester in solvents”, *Journal of Chemical Physics*, vol. 137, 244308, 2012
  32. S. Banerjee, “Molecular simulation of the self-agglomeration of carbon nanostructures in various chemical environments”, *Proceedings of IMECE 2012*, ASME IMECE, Houston, 2012
  33. S. Banerjee, and H. Briesen, “Molecular dynamics simulations of glycine crystal-solution interface”, *Journal of Chemical Physics*, vol. 131, 184705, 2009 (Selected for publication in the November 15, 2009 issue of the Virtual Journal of Biological Physics Research)
  34. G. Balasubramanian, S. Banerjee, and I.K. Puri, “Unsteady nanoscale thermal transport across a solid-fluid interface”, *Journal of Applied Physics*, vol. 104, 064306, 2008 (Selected for publication in the October 6<sup>th</sup>, 2008 issue of the Virtual Journal of Nanoscale Science & Technology)
  35. G. Balasubramanian, S. Banerjee, and I.K. Puri, “Interfacial thermal resistance in nanoscale heat transfer”, *Proceedings of IMECE 2008*, ASME IMECE, Boston, 2008
  36. S. Banerjee, S. Naha, and I.K. Puri, “Molecular simulation of growth mode during catalytic synthesis of carbon nanotubes”, *Applied Physics Letters*, vol. 92, 233121, 2008 (Selected for publication in the June 30<sup>th</sup>, 2008 issue of the Virtual Journal of Nanoscale Science and Technology)
  37. S. Banerjee, and I.K. Puri, “Enhancement in hydrogen storage in carbon nanotubes under modified conditions”, *Nanotechnology*, vol. 19, 155702, 2008
  38. S. Banerjee, S. Murad and I.K. Puri, “preferential ion and water intake using charged

- carbon nanotubes”, *Chemical Physics Letters*, vol. 434, pp. 292-296, 2007
39. S. Banerjee, S. Murad and I.K. Puri, “Hydrogen storage in carbon nanostructures: possibilities and challenges for fundamental molecular simulations”, *Proceedings of the IEEE*, vol. 94(10), pp. 1806-1814, 2006
  40. S. Banerjee, S. Murad, and I.K. Puri, “Carbon nanotubes as nano-pumps: a molecular dynamics investigation”, *Proceedings of ASME ICNMM2006*, Fourth International Conference on Nanochannels, Microchannels and Minichannels, Limerick, Ireland, 2006
  41. S. Banerjee, D. Sanyal, S. Sen, and I.K. Puri, “A methodology to control direct-fired furnaces”, *International Journal of Heat and Mass Transfer*, vol. 47(24), pp. 5247-5256, 2004
  42. S. Banerjee, S. Sen, I.K. Puri, and S. Sanyal, “Control strategy for direct fired furnaces”, 3rd Joint Technical Meeting of the US Sections of The Combustion Institute, *Paper PG12*, Chicago, 2003

#### BOOK CHAPTER

43. SM Mortuza and S. Banerjee, “Organic Solar Cells: Materials, Devices, Interfaces and Modeling”, Edited by: Qiquan Qiao, Publisher: *CRC Press*, ISBN 9781482229837, 2015

#### PRESENTATIONS AT CONFERENCES (Presenter Underlined)

44. R. Khanal, S. Briggs, N. Ayers, T. Mohammad, S. Banerjee and S. Choudhury, “Comparison of bulk, surface, and interfacial properties in organic halide perovskite for photovoltaic applications”, to be presented, MRS Fall Meeting, Boston, 2017
45. A. Dive, C. C. King, S. W. Martin, S. P. Beckman, and S. Banerjee, “Modeling structure and properties of Na<sub>2</sub>S based glassy electrolytes”, to be presented, ASME IMECE, Tampa, 2017
46. M.F.N. Taufique, R. Khanal, S. Choudhury, and S. Banerjee, “Modeling-based study of structural and electronic properties of methyl ammonium lead iodide perovskite surfaces relevant to solar cells”, to be presented, ASME IMECE, Tampa, 2017
47. A. Dive, C. King, S. Beckman, S. Martin, and S. Banerjee, “Modeling Na<sub>2</sub>S based glassy electrolytes for high performance solid state sodium ion batteries”, 231st ECS Meeting, New Orleans, LA, 2017
48. A. Dive, Min-Kyu Song, and S. Banerjee, “Model based evaluation of graphene oxide (GO)/Sulfur composite cathodes for high performance Li-S batteries”, 231st ECS Meeting, New Orleans, LA, 2017
49. A. Dive, C. King, S. Beckman, and S. Banerjee, “Molecular dynamics simulations of glassy solid electrolytes for sodium ion batteries”, MRS Spring Meeting, Phoenix, 2017
50. M.F.N. Taufique, S.M. Mortuza, A. Dive and S. Banerjee., “Modeling the growth mechanism and morphology of solution-processed monolayers on perovskite surfaces for solar cell applications”, MRS Spring Meeting, Phoenix, 2017 (**Nominated for Best Poster Award**)
51. S. Beckman, A. Dive, C. King, S. Martin, S. Banerjee, “Multi-scale simulations of Na<sub>2</sub>S + SiS<sub>2</sub> glassy electrolyte”, *Bulletin of the American Physical Society*, 62, 2017
52. M.F.N. Taufique, S.M. Mortuza, and S. Banerjee, “Multiscale modeling based study of solution processed deposition of electron transport layers on perovskite crystal surface”, ASME IMECE, Phoenix, 2016

53. A. Dive, C. King, S. Beckman, S. Martin, and S. Banerjee, “Molecular dynamics simulations of glassy solid electrolytes for sodium ion batteries”, ASME IMECE, Phoenix, 2016
54. C. King, A.M. Dive, S.W. Martin, S.P. Beckman and S. Banerjee, “Molecular dynamics simulations of Na<sub>2</sub>S + SiS<sub>2</sub> glassy solid electrolytes”, Materials Science & Technology 2016, Salt Lake City, Utah, 2016
55. S. Banerjee, “Designing molecularly-tailored electrolytes for next-generation lithium batteries”, Theory and Application of Computational Chemistry – TACC2016, Seattle, 2016
56. A. Dive, and S. Banerjee, “A molecular dynamics study of graphene oxide (GO)/sulfur composite cathodes for Li-S batteries”, ECS’ 18<sup>th</sup> International Meeting on Lithium Batteries, Chicago, 2016
57. S. Banerjee, “Multiscale modeling towards design of molecularly-tailored electrolytes”, NSF-IUSSTF Workshop on Analysis of Multiphysics Phenomena in Li-ion Cells held in Indian Institute of Technology, Bombay, 2016
58. A. Dive, R. Gonzalez, and S. Banerjee, “Graphene oxide-sulfur composite cathodes for high performance Li-S batteries: A molecular dynamics study”, MRS Spring Meeting, Phoenix, 2016
59. S.M. Mortuza, M.F.N. Taufique, and S. Banerjee, “Modeling deposition of [6,6]-phenyl-C61-butyric acid methyl ester based electron transport layer on perovskite crystal surface”, MRS Spring Meeting, Phoenix, 2016
60. R. Gonzalez, A. Dive, and S. Banerjee, “Modeling Next Generation Lithium-Sulfur Batteries”, LSAMP Conference, Seattle 2016 (**Best Poster Award**)
61. I. Dutta, B. Talebanpour, S. Bhassyvasantha, L. Meinshausen, S. Banerjee, B. Majumdar, “Mitigation of Sn whisker growth by dopant addition”, 2016 TMS Annual Meeting & Exhibition, Nashville, 2016
62. L. Meinshausen, A. Buckel, S. Banerjee, I. Dutta, B. Majumdar, “Sn Whisker Mitigation Studies Using Dopant Additions”, Materials Science & Technology 2015, Columbus, OH, 2015
63. SM Mortuza and S. Banerjee, “A novel multiscale model for agglomeration of nanoparticles during solvent based processing of thin nanocomposite films”, ASME IMECE, Houston, 2015
64. SM Mortuza, and S. Banerjee, “Self-assembled molecular aggregates during solution-processing of thin films”, ASME IMECE, Houston, 2015
65. SM Mortuza, L. Kariyawasam and S. Banerjee, “Solution Based Processing of Nanoparticles Relevant to Organic Electronics: A Modeling Based Study”, ASME Applied Mechanics and Materials Conference, Seattle, 2015 (**Graduate student SM Mortuza won travel award from the National Science Foundation to present this poster**)
66. SM Mortuza, and S. Banerjee, “Modeling the self-assembly of nanoparticles in solvents based on molecular dynamics and kinetic Monte Carlo: A novel approach”, AIChE Annual Meeting, Salt Lake City, 2015
67. S. Banerjee, and P. Dutta, “Electron transfer reactions at the anode-electrolyte interface in lithium-air batteries – a first principles study”, ASME Applied Mechanics and Materials Conference, Seattle, 2015 (Presented by: Aniruddha Dive)

68. S.M. Golam Mortuza and S. Banerjee, "Understanding self-assembly of organic nanoparticles during solution processing of thin films", ASME Applied Mechanics and Materials Conference, Seattle, 2015
69. S.M. Mortuza and S. Banerjee, "Modeling electrophoretic alignment and deposition of carbon nanotubes on substrates", ASME Applied Mechanics and Materials Conference, Seattle, 2015
70. S. Mortuza, and S. Banerjee, "Multi-scale modeling of nanoparticle aggregation during solution processing of photoactive layers", MRS Spring Meeting, San Francisco, 2015
71. S. Kazemiabnavi, P. Dutta, and S. Banerjee, "Theoretical investigation of the electron transfer reaction at the cathode-electrolyte interface in lithium-air battery", MRS Spring Meeting, San Francisco, 2015
72. SM Mortuza, and S. Banerjee, "Modeling fullerene aggregation in electrolyte solutions: A combined deterministic-stochastic framework", 249th ACS National Meeting & Exposition, Denver, 2015
73. L.M. Meinshausen, S. Banerjee, I. Dutta, B. Majumdar, A. Buckel, "Effect of solute addition and grain structure modification on boundary diffusion and whisker growth in tin coatings", 2015 TMS Annual Meeting & Exhibition, Orlando, FL, 2015
74. S.M. Mortuza, and S. Banerjee, "Molecular modeling study of benzo dithiophene based polymers and organic nanoparticles for organic photovoltaic solar cells", 247th ACS National Meeting & Exposition, Dallas, 2014
75. M. Mostafa, and S. Banerjee, "Molecular dynamics study of electrophoretic alignment of carbon nanotubes and their deposition on substrates", 247th ACS National Meeting & Exposition, Dallas, 2014
76. S.M. Mortuza, and S. Banerjee, "Modeling of nanoparticles and conjugated polymers in aromatic solvents to mimic synthesis of photoactive layers of organic photovoltaic solar cells", ASME IMECE 2013, San Diego, 2013
77. S. Banerjee, "Modeling ionic liquid based electrolytes for lithium batteries", ASME IMECE 2013, ASME IMECE, San Diego, 2013
78. A. Deshpande, J. Avila, and S. Banerjee, "Evaluation of the Ionic Conductivity of Nitrile-Based Liquid Electrolytes for Lithium-ion Batteries", ASME IMECE 2013, ASME IMECE, San Diego, 2013
79. S.M. Mortuza, M. Bartolo, and S. Banerjee, "Molecular modeling of nanoparticles and conjugated polymers during synthesis of photoactive layers of organic photovoltaic solar cells", AIChE Annual Meeting, San Francisco, 2013
80. D. Binion, and S. Banerjee, "Modeling-based study of the effect of diluents on transport properties of ionic liquid electrolytes", MRS Spring Meeting, San Francisco, 2013
81. S.M. Mortuza, and S. Banerjee, "Molecular association of [6,6]-phenyl-C61-butyric acid methyl esters (PCBM) with conjugated polymers relevant to organic photovoltaic cells", MRS Spring Meeting, San Francisco, 2013
82. S.M. Mortuza, and S. Banerjee, "Molecular morphology of acceptor nanoparticles in organic photovoltaic solar cells", ASME IMECE 2012, ASME IMECE, Houston, 2012

83. S.M. Golam Mortuza, and S. Banerjee, "Molecular simulation of nanoparticle-polymer systems relevant to organic photovoltaic solar cells", FOMMS meeting, Mt. Hood, Oregon, 2012
84. A. Voigt, S. Banerjee, and H. Briesen, "A Multiscale Simulation Model to Simulate Crystal Growth", Poster at the 40th BACG conference, 04.-06.09.2009, Bristol/UK.
85. S. Banerjee, and H. Briesen, "Multiscale Simulation of Crystal Growth", Jahrestreffen der ProcessNet Fachausschüsse Kristallisation und Fluidverfahrenstechnik, Dortmund, March 2009
86. S. Banerjee, S. Naha, and I.K. Puri, "A Numerical Prediction of Growth Mode during Catalytic Synthesis of Carbon Nanotubes", The Mechanics Conference to Celebrate the 100<sup>th</sup> Anniversary of The Department of Engineering Science and Mechanics, Virginia Tech, Blacksburg, 2008
87. G. Balasubramanian, S. Banerjee, and I.K. Puri, "Molecular Dynamics Investigation of Interfacial Heat Transfer at the Nanoscale", The Mechanics Conference to Celebrate the 100<sup>th</sup> Anniversary of The Department of Engineering Science and Mechanics, Virginia Tech, Blacksburg, 2008
88. S. Banerjee, and I.K. Puri, "Hydrogen Transport and Storage Inside Carbon Nanotubes in Presence of Encapsulated Metal Ions", 60<sup>th</sup> Annual Meeting of the APS DFD, Salt Lake City, 2007
89. S. Banerjee, S. Murad and I.K. Puri, "Influence of Electrostatic Field on Storage of Hydrogen in Carbon Nanotubes", Paper # Q20.49, MRS Fall Meeting, Boston, 2006
90. S. Naha, S. Banerjee, and I.K. Puri, "A Multiscale Approach to the Modeling and Analysis of Growth Rate of Carbon Nanostructures" The 43rd Annual Technical Meeting of the Society of Engineering Science, University Park, Pennsylvania, 2006
91. S. Banerjee, S. Murad, and I.K. Puri, "Molecular Dynamics Investigation of Ionic Flow and Separation by Carbon Nanotube Electrodes", American Physical Society Division of Fluid Dynamics Meeting, Chicago, 2005

#### **OTHER PRESENTATIONS**

92. S. Banerjee, Modeling based design of materials for next-generation energy conversion and storage devices, CIRC Workshop, WSU, 2017
93. M.F.N. Taufique, S.M. Mortuza, and S. Banerjee., "Modeling the growth mechanism and morphology of solution-processed monolayers on perovskite surfaces for solar cell applications", MME Student Day, 2017
94. M.F.N. Taufique, S.M. Mortuza, and S. Banerjee, "Modeling deposition of [6,6]-phenyl-C61-butyric acid methyl ester based electron transport layer on perovskite crystal surface", MME Student Day, 2016
95. R. Gonzalez, A. Dive, and S. Banerjee, "Modeling Next Generation Lithium-Sulfur Batteries", SURCA 2016, WSU
96. M.F.N. Taufique, S.M. Mortuza, and S. Banerjee, "Modeling of solution processed [6,6]-phenyl-C61-butyric acid methyl ester thin films deposition on perovskite crystal surface", MSEP Research Exposition, Pullman, 2016
97. SM Mortuza and S. Banerjee, "Molecular association of [6,6]-phenyl-C61-butyric acid methyl esters (PCBM) with conjugated polymers relevant to organic photovoltaic cells",



- MSEP Research Exposition, Pullman, 2015
98. Saeed Kazemiabnavi, and Soumik Banerjee, "Ab initio Modeling of Reaction Rates at Electrode-Electrolyte Interfaces of Lithium-Air Batteries", MME Student Day, 2014
  99. Saeed Kazemiabnavi, Kisoo Yoo, Anirudh Deshpande, Prashanta Dutta, and Soumik Banerjee, "Design of Molecularly Tailored Electrolytes for High Performance Lithium Batteries" JCATI Research Symposium, Pullman, WA, April 2014
  100. S.M. Mortuza and S. Banerjee, "Identifying novel materials for organic photovoltaic solar cells using molecular simulations", 3M Science and Engineering Faculty Day, Minneapolis, 2013
  101. S. Banerjee, and H. Briesen, "Molecular Dynamics Simulation of Crystal Growth", Max-Planck Institute Evaluation, Magdeburg, Germany, 2009
  102. S. Banerjee, and H. Briesen, "Multiscale Simulation of Crystal Growth", PCP Workshop, Bad Harzburg, Germany, 2008
  103. S. Banerjee, and I.K. Puri, "Hydrogen Transport and Storage Inside Carbon Nanotubes in Presence of Encapsulated Metal Ions", Fall Fluid Mechanics Symposium, Virginia Tech, 2007
  104. S. Banerjee, S. Naha, and I.K. Puri, "Synthesis of Carbon Nanotubes and their Hydrogen Storage Capacity", 2006 Dean's Forum on Energy Security and Sustainability, Virginia Tech, 2006

#### TEACHING APPOINTMENTS AND RESPONSIBILITIES

- Instructor, Fundamentals of Engineering Examination Review (ME 466) – Thermodynamics/Heat Transfer components, School of Mechanical and Materials Engineering, Washington State University, Fall 2015, Spring 2016, Fall 2016, Spring 2017
- Instructor, Heat Transfer (ME 404/ME 304), School of Mechanical and Materials Engineering, Washington State University, Fall 2013, Spring 2014, Spring 2015, Fall 2015, Spring 2016, Fall 2017, Spring 2018
- Co-Instructor, Microscopic Analysis of Solid Surfaces (MatSci 571), Materials Science, Washington State University, Spring 2013
- Instructor, Statistical Thermodynamics (ME 526), School of Mechanical and Materials Engineering, Washington State University, Spring 2013, Spring 2015, Spring 2017
- Instructor, Fundamentals of Thermodynamics (ME 301), School of Mechanical and Materials Engineering, Washington State University, Fall 2011, Fall 2012, Spring 2013, Fall 2014, Fall 2016, Spring 2017, Spring 2018
- Instructor, Advanced Heat Transfer (ME 515), School of Mechanical and Materials Engineering, Washington State University, Spring 2012
- Co-instructor, Thermodynamics II (MECHENG 336), Department of Mechanical Engineering, University of Michigan – Ann Arbor, Fall 2010
- Instructor, Fluid Mechanics Laboratory (ESM 3034), Department of Engineering Science and Mechanics, Virginia Tech, Spring 2006, Spring 2007 and Spring 2008
- Teaching Assistant, Dynamics (ESM 2304), Department of Engineering Science and Mechanics, Virginia Tech, Summer 2007
- Teaching Assistant, Statics (ESM 2204), Department of Engineering Science and Mechanics, Virginia Tech, Fall 2005, Spring 2005 and Fall 2004

## MENTORING ACTIVITIES

- Graduate student Mohammad Taufique, PhD in Materials Science and Engineering, Washington State University, 2015-present, working on multi-scale modeling of deposition of electron transport layer on methyl ammonium lead halide perovskite
- Graduate student Aniruddha Dive, PhD in Mechanical Engineering, Washington State University, 2015-present, working on modeling solid-state sodium ion batteries and graphene oxide based cathode support for lithium sulfur batteries
- Graduate student Saeed Kazemiabnavi, PhD in Materials Science and Engineering, Washington State University, 2013-2014, *Currently at University of Michigan*, worked on modeling ionic liquid electrolytes and electrode-electrolyte interfaces for lithium-air batteries
- Graduate student Anirudh Deshpande, MS in Mechanical Engineering, Washington State University, 2013-2014, *Currently employed at Ford*, worked on modeling ionic liquid electrolytes for lithium-air batteries
- Graduate student Mohammad Mostafa, MS in College of Engineering, Washington State University, 2013-2014, worked on modeling electrophoretic deposition of carbon nanotubes
- Graduate student S.M. Golam Mortuza, PhD in Mechanical Engineering, Washington State University, 2012-present, *Currently postdoc at University of Michigan*, worked on aggregation and deposition of carbon nanoparticles relevant to thin film photovoltaics, won *NSF travel grant to attend ASME's McMat Conference in 2015*, selected for an internship as part of Lawrence Livermore National Laboratory's prestigious 2015 Computational Chemistry and Materials Science Summer Institute, won *Research Excellence Award from the GPSA at WSU*, MME Outstanding Researcher Award in Spring 2015, MME Outstanding TA Award in Spring 2016, Voiland College of Engineering & Architecture Outstanding TA Award in Spring 2016
- Undergraduate students Jonathan Gilvey, Corinna Cisneros, Mark Bartolo and Jose Avila, NSF REU program
- Undergraduate student Corinna Cisneros, through NSF REU Program and Louis-Stokes Alliance for Minority Participation (LSAMP) Program, Washington State University, 2011-2013, *Currently employed at Boeing*
- Undergraduate student Joshua Powers, Washington State University, 2012-2013, *Currently employed at Columbia Helicopters*
- Undergraduate student Lahiru Kariyawasam, Washington State University, 2012-2015, *Currently pursuing PhD in Physics at Northeastern University*

## PROFESSIONAL SERVICE AND OUTREACH

### Outreach

- Advised two students, from under-represented minority community, on research projects as part of NSF's REU program in summer 2013. The research efforts of one of the students resulted in publication of a paper in the *Proceedings of the American Institute of Chemical Engineers' Annual Meeting* at San Francisco in 2013. Inspired by research experience at WSU, one of the students is pursuing PhD. The other student's

work was presented at the American Society of Mechanical Engineers' annual conference at San Diego in 2013. He moved to WSU in 2014 and is currently pursuing a major in Mechanical Engineering at WSU

- Served as judge for the high school science competition *Imagine Tomorrow* for students in the states of Washington, Idaho, Montana, or Oregon, 2012 and 2013
- Advised 4 undergraduate students in NSF's REU program in Summer 2012, 2013, and 2014

#### **Book Reviewer**

- CRC Press
- Springer

#### **Proposal Review Panel**

- Participated in panel review for the NSF, 2014, 2015, 2016 & 2017
- Participated in a virtual review panel for Department of Energy SCGF Program, 2012

#### **Participation as Judge**

- Served as judge for the MRS Micrograph Contest, Northwest Region, WSU, 2014
- Served as judge for the NSF-supported poster symposium at the ASME IMECE 2013 congress
- Served as judge at Showcase for Undergraduate Research and Creative Activities (SURCA) event at Washington State University, 2012 and 2013
- Served as judge for Paul E. Torgersen Award for Graduate Research Excellence, Virginia Tech, Spring 2006

#### **Membership of Professional Organizations**

- American Society of Mechanical Engineers (ASME)
- Materials Research Society (MRS)
- American Chemical Society (ACS)
- American Society for Engineering Education (ASEE)
- American Institute of Chemical Engineers (AIChE)

#### **Participation in Committees at Professional Organizations**

- Chair, *ASME committee for Electrochemical Energy Conversion and Storage*, 2016 - present
- Member, *Nanoengineering for Energy and Sustainability ASME Group*, 2012 – present
- Member, *ASME Technical Committee on Nanomaterials for Energy*, 2015 – present

#### **Symposium Organizer**

- Topic organizer for "Fuel Cell Systems Design and Applications" with multiple sessions at ASME IMECE, Tampa, 2017
- Topic organizer for "Electrochemical Energy Conversion and Storage" with multiple sessions at ASME IMECE, Tampa, 2017
- Topic organizer for "Electrochemical Energy Conversion and Storage" with multiple sessions at ASME IMECE, Phoenix, 2016
- Track organizer for conference-wide poster session, ASME 2016 Power and Energy

Conference, Charlotte, 2016

- Organized symposium on Computational Nanotechnology with 4 sessions and 3 invited keynote speakers at ASME's Applied Mechanics and Materials Conference (McMat), Seattle, 2015

### Session Chair

- Chaired session on "Electrochemical Energy Conversion and Storage" at ASME IMECE, 2016
- Chaired session on "Methods" at the Theory and Applications of Computational Chemistry (TACC) Conference, Seattle, 2016
- Chaired session on "Modeling and Materials" at the NSF-IUSSTF Workshop on Multiscale Analysis of Li Ion Cells at Indian Institute of Technology, Mumbai
- Selected to serve as chair for the session on "Basic Research in Colloids, Surfactants and Nanomaterial" at 2015 Spring ACS National Meeting in Denver, CO
- Selected to serve as co-chair for the session on "Advanced Electrochemical Storage Concepts" at ASME IMECE, 2013

### Journal Reviewer

*Scientific Reports*

*Journal of Chemical Physics*

*Journal of Physical Chemistry B*

*Journal of Physical Chemistry C*

*Journal of Membrane Science*

*Journal of Physical Chemistry Letters*

*Physical Chemistry Chemical Physics*

*Journal of the Electrochemical Society*

*Journal of Chemical Physics*

*Materials Science and Engineering B*

*Computational Materials Science*

*Journal of Nanoscience and Nanotechnology*

*IEEE Transactions on Electron Devices*

*ACS Applied Materials and Interfaces*

*Journal of Electrochemical Energy Conversion and Storage*

*Nanoscale and Microscale Thermophysical Engineering*

*ASME Power & Energy*

*Proceedings of the ASEE*

*Nature Chemistry*

*Nanoscale*

*Macromolecules*

*Soft Matter*

*Physica A*

*Crystal Growth and Design*

*Materials Chemistry A*

*Journal of Power Sources*

*Nano Energy*

*Materials*

*Nanotechnology Review*

*Langmuir*

*Physica E*

*Journal of Heat Transfer*

*Journal of Fluids Engineering*

*Journal of Molecular Liquids*

*RSC Advances*

*Small*

### Learning Modules for REU Students

- Presented learning module on Multiscale Modeling of Materials for REU students, Summer 2012, Summer 2013 and Summer 2014

### Participation in Committees at WSU

- Web & External Communication Committee, School of Mechanical and Materials Engineering, Washington State University, Fall 2017 - present
- High performance computing (HPC) committee, Voiland College of Engineering and

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Architecture, Fall 2016 - present

- Faculty Search Committee – Computational Materials Science, School of Mechanical and Materials Engineering, Washington State University, 2015
- Committee to revise MSEP Graduate Handbook, Materials Science and Engineering Program, Washington State University, 2014
- Graduate Studies Committee, School of Mechanical and Materials Engineering, Washington State University, 2012 – 2013; 2014 - present
- Broad Faculty Search Committee, School of Mechanical and Materials Engineering, Washington State University, 2014
- Faculty Search Committee, School of Mechanical and Materials Engineering, Washington State University, 2013 – 2014
- Computing Tools Committee, School of Mechanical and Materials Engineering, Washington State University, 2011 - 2012