

# Badri Narayanan

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Theory & Modeling Group  
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## EDUCATION

- Colorado School of Mines**, Golden, Colorado, USA **2013**  
*Ph. D., Materials Science*  
Dissertation: Understanding structure-property relationships in  $\beta$ -eucryptite through atomistic simulations  
Advisors: Prof. Cristian V. Ciobanu & Prof. Ivar E. Reimanis
- Indian Institute of Science**, Bangalore, India **2008**  
*Masters in Engineering, Materials Engineering*  
Dissertation: Microstructural evolution in alloy thin films  
Advisor: Prof. Thennathur A. Abinandanan
- National Institute of Technology Karnataka**, Surathkal, India **2006**  
*Bachelors in Engineering, Metallurgical and Materials Engineering*

## RESEARCH INTERESTS

- Structure-property relationships and atomistic understanding of novel materials/interfaces for energy applications including catalysis, tribology, devices and corrosion.
- Development of reactive empirical potentials to facilitate large-scale molecular dynamics simulations for a wide range of materials systems including metal clusters, 2D materials, oxides and nitrides.
- Self-assembly of bio-materials, and ligand decorated nanoparticles for energy and device applications at mesoscale

## RESEARCH EXPERIENCE

- Argonne National Laboratory**, Argonne, IL, USA **April 2014 – present**  
*Nanoscience & Technology Division*  
*Postdoctoral Fellow*  
Advisor: Dr. Subramanian K. R. S. Sankaranarayanan
- Developed empirical potential models for accurate atomistic simulations of reactive interfaces for energy applications. Special emphasis on metal nanoclusters, oxides, carbides, nitrides, 2D materials beyond graphene, and Li-Si interfaces.
  - Developed computational workflow for seamlessly employing classical molecular dynamics (MD) and electronic structure calculations to investigate electronic transport properties in metal/oxide/nitride interfaces.
  - Investigated structure-property relationships at various atomic interfaces relevant for catalysis, tribology, and large-area synthesis of 2D materials using multi-million atom reactive MD simulations, and electronic structure calculations
  - Investigated directed self-assembly of organic molecules, polymers, and ligand-decorated metal nano-particle superlattices using coarse-grained MD simulations
- Colorado School of Mines**, Golden, CO, USA **Sep. 2013 – Mar. 2014**  
*Department of Mechanical Engineering*  
*Postdoctoral Research Fellow*  
Advisor: Prof. Cristian V. Ciobanu

- Developed a microscopic model of Type I collagen molecules, and used it to show that the morphology of self-assembled collagen on flat substrates is primarily governed by the competition between collagen-collagen and collagen-substrate interactions.
- Assisted in developing and writing research grant proposals for NSF and other agencies

**Colorado School of Mines**, Golden, CO, USA

**Aug. 2008 – Aug. 2013**

*Department of Metallurgical & Materials Engineering*

*Graduate Research Assistant*

Advisors: Prof. Cristian V. Ciobanu and Prof. Ivar E. Reimanis

- Resolved long-standing controversy in the literature surrounding the sign of linear compressibility of lithium aluminum silicates using density functional theory (DFT) calculations.
- Parameterized a reactive force field (ReaxFF) for describing the atomic interactions Li-Al-Si-O systems by using DFT calculated structural and thermodynamic properties of numerous bulk phases of oxides, silicates, and aluminates, as well as several representative clusters.
- Investigated atomic-scale mechanisms underlying radiation tolerance and pressure-induced structural transitions in  $\beta$ -eucryptite using ReaxFF based molecular dynamics (MD) simulations.
- Discovered that carbon monoxide can remove all major oxygen-containing functional groups on graphene oxide at moderate temperatures by employing DFT calculations and MD simulations.
- Identified a novel migration mechanism of atomic hydrogen in porous carbon using DFT-based nudged elastic band calculations. This mechanism involves hopping of H atoms from one carbon nanotube to another, and explains empirically observed fast kinetics of H in porous carbon.

**Indian Institute of Science**, Bangalore, India

**Aug. 2006 – Aug. 2008**

*Department of Metallurgical & Materials Engineering*

*Graduate Research Assistant*

Advisor: Prof. Thennathur A. Abinandanan

- Developed a phase-field model to describe growth of binary alloy thin films that exhibit spinodal decomposition.
- Employed this phase-field model to explain microstructural evolution in binary alloy thin films in terms of the interplay between the deposition rate and the timescale associated with spinodal decomposition.

## **AWARDS**

- Best student presentation in the Annual Conference of Colorado Center for Advanced Ceramics (2010, 2012).
- K.K. Malik Award for best masters thesis in materials science, Indian Institute of Science (2008)
- Best oral presentation in the National Metallurgist Day--Indian Institute of Metals Technical Meeting (2007)
- National Merit Scholarship from the Ministry of Human Resources Development, Indian Institute of Science, India (2006-2008)
- Merit Certificate in Science and scholarship from the Central Board of Secondary Education for outstanding performance (placed in top 0.1% students) in All India Secondary School Examination (2000)

## **TEACHING & MENTORING EXPERIENCE**

**Argonne National Laboratory**, Argonne, IL, USA

*Graduate Student Mentoring*

- Amir Al Khatib, Electrical Engineering, Northern Illinois University
- Henry Chan, Department of Chemistry, University of Illinois, Chicago

**Since Apr. 2015**

**Since Sep. 2015**

*Undergraduate Student Mentoring*

- Karen Zheng, Engineering, University of Illinois Urbana-Champaign

**Jun. 2015 – Aug. 2015**

Colorado School of Mines, Golden, CO, USA

Guest Lecturer

- Ceramic Engineering

Fall 2012

Teaching Assistant

- Electronic Properties of Materials
- Ceramic Engineering
- Nanomechanical Measurements
- Processing of Ceramics

Spring 2009, Spring 2011

Fall 2009, Fall 2010

Fall 2011

Spring 2012

## PROFESSIONAL SERVICES

- Referee for Physical Review B, Nanotechnology, Physical Chemistry Chemical Physics, Journal of Physics Condensed Matter, RSC Advances, Journal of Physics D, Physics Letters A
- Develop user-friendly materials modeling tools that are disseminated to the computational materials research community via the user facility at Argonne
- Member of Materials Research Society, American Ceramics Society, American Society for Metals, The Minerals, Metals & Materials Society and American Vacuum Society.

## PUBLICATIONS

Manuscripts under review

1. **B. Narayanan**, A. Kinaci, F. Sen, M. J. Davis, S. Gray, M. K Y. Chan, and S. Sankaranarayanan  
*Describing the diverse geometries of gold from nanoclusters to bulk – a first-principles based hybrid bond order potential*  
Journal of Chemical Theory and Computation (2015)
2. A. Kinaci, **B. Narayanan**, F. Sen, M. Davis, S. Gray, S. Sankaranarayanan, and M. Chan  
*Evolutionary algorithm search for global minimum structures of Au nano-clusters*  
Nanoscale (2015)
3. D. Berman, S. Deshmukh, **B. Narayanan**, S. Sankaranarayanan, Z. Yan, A. Baladin, A. Zinovev, D. Rosenmann, and A. Sumant  
*Metal induced ultra-fast transformation of diamond into single domain graphene on wafer scale*  
Nature Communications (2015)
4. S. Das, M. Bera, S. Tong, **B. Narayanan**, G. Kamath, A. Mane, M. Antonio, S. Sankaranarayanan and A. Roelofs  
*A Self-Limiting Electro-Ablation Technique for the Top-Down Synthesis of Large Area Monolayers of 2D Materials*  
ACS Nano (2015)
5. A. Eridemir, G. Ramirez, **B. Narayanan**, O. Eryilmaz, Y. Liao, and S. K. R. S. Sankaranarayanan  
*Carbon-based protective tribofilms from lubricating oils*  
Nature (2015)

Manuscripts published

6. **(Invited) B. Narayanan**, S. Deshmukh, S. Sankaranarayanan, and S. Ramanathan  
*Strong correlations between structural order and passive state at water–copper oxide interfaces*  
Electrochimica Acta 179, 386 (2015)
7. F. Sen, A. Kinaci, **B. Narayanan**, S. Gray, M. Davis, S. Sankaranarayanan, M. Chan  
*Towards accurate prediction of catalytic activity in IrO<sub>2</sub> nanoclusters via first principles-based variable charge force field*  
Journal of Materials Chemistry A 37, 18970 (2015)
8. S. A. Deshmukh, **B. Narayanan**, G. Kamath, V. Pol, J. Wen, D. Miller, and S. Sankaranarayanan  
*Nanoscale origin and evolution of kinetically induced defects in carbon spheres*

- Carbon 96, 647 (2015)
9. G. Kamath, **B. Narayanan**, and S. Sankaranarayanan  
*Atomistic origin of superior performance of ionic liquid electrolytes for Al-ion batteries*  
Physical Chemistry Chemical Physics 16, 20387 (2014)
  10. A. Ebnonnasir, **B. Narayanan**, S. Kodambaka, and C.V. Ciobanu  
*Controlling bandgap of single layer MoS<sub>2</sub> in graphene/MoS<sub>2</sub> heterostructures*  
Applied Physics Letters 105, 031603 (2014)
  11. **B. Narayanan**, G. Gilmer, J. Tao, J. DeYoreo, and C. Ciobanu  
*Self-assembly of collagen on surfaces: the interplay of collagen-collagen and collagen-substrate interactions*  
Langmuir 30, 1343 (2014)
  12. **B. Narayanan**, I. Reimanis, and C. Ciobanu  
*Atomic-scale mechanism for pressure-induced amorphization of  $\beta$ -eucryptite*  
Journal of Applied Physics 114, 083520 (2013)
  13. **B. Narayanan**, S. Weeks, B. Jariwala, B. Macco, J. -W. Weber, S. Rathi, M. van de Sanden, P. Sutter, S. Agarwal and C. V. Ciobanu  
*Carbon monoxide induced reduction and healing of graphene oxide*  
Journal of Vacuum Science and Technology A 31, 040601 (2013)  
**Featured on the cover of the July 2013 issue of Journal of Vacuum Society and Technology A**  
**Featured in the Research Highlights of American Vacuum Society (June 2013)**
  14. **B. Narayanan**, I. Reimanis, H. Huang and C. Ciobanu  
*Radiation effects and tolerance mechanism in  $\beta$ -eucryptite*  
Journal of Applied Physics 113, 033504 (2013)
  15. **B. Narayanan**, Y. Zhao and C. Ciobanu  
*Migration mechanism for atomic hydrogen in porous carbon materials*  
Applied Physics Letters 100, 203901 (2012)
  16. **B. Narayanan**, A. van Duin, B. Kappes, I. Reimanis, and C. Ciobanu  
*A reactive force field for lithium–aluminum silicates with applications to eucryptite phases*  
Modelling and Simulation in Materials Science and Engineering 20, 015002 (2012)
  17. **B. Narayanan**, I. Reimanis, E. Fuller, Jr. and C. Ciobanu  
*Elastic constants of  $\beta$ -eucryptite studied by density functional theory*  
Physical Review B 81, 104106 (2010).

## CONFERENCE TALKS

1. **B. Narayanan**, S. Deshmukh, G. Kamath, E. Shevchenko, and S. Sankaranarayanan  
*Role of ligand dynamics in structural stability and pressure behavior of supercrystals self-assembled from crystalline nanoparticles*  
Materials Research Society Fall Meeting, Boston MA, December 2015 (Accepted)
2. **B. Narayanan**, F.Sen, A. Kinaci, Z. Mei, M. J. Davis, S. Gray, M. Chan, and S. Sankaranarayanan  
*Evolutionary strategy for developing interatomic potentials to bridge the electronic and atomistic length scales*  
Materials Research Society Fall Meeting, Boston MA, December 2015 (Accepted)
3. **(Invited) B. Narayanan**, H. Huang, A.van Duin, C. Ciobanu, and I. Reimanis  
*Structure-property relationships in  $\beta$ -eucryptite*  
Materials Science and Technology Conference, Pittsburgh October 2014
4. **B. Narayanan**, A. Kinaci, M. J. Davis, M. Chan, S. Sankaranarayanan, and S. Gray, *Development of novel force field for gold nanoclusters*, Materials Science and Technology Conference, Pittsburgh, October 2014
5. **B. Narayanan**, A. Kinaci, F.Sen, M. J. Davis, M. Chan, S. Sankaranarayanan, and S. Gray

- A Novel Empirical Force Field to Capture Size-Dependent Dimensionality Effects in Au Nanoclusters*  
Electrochemical Society Meeting, Chicago May 2015
6. **B. Narayanan**, S. Deshmukh, S. Sankaranarayanan, and S. Ramanathan  
*Atomistic Insights into the Interaction of Copper Oxide Surfaces with Chloride Ions in Aqueous Media*  
Electrochemical Society Meeting, Chicago May 2015
  7. **B. Narayanan**, I. Reimanis, and C. Ciobanu  
*Understanding structure-property relationships in  $\beta$ -eucryptite through atomistic simulations*  
Materials Research Society Fall Meeting, Boston MA, December 2013.
  8. **B. Narayanan**, G. Gilmer, J. de Yoreo, and C. Ciobanu  
*Assembly of collagen on surfaces: insights from molecular simulations*  
Materials Research Society Fall Meeting, Boston MA, December 2013.
  9. **B. Narayanan**, S. Weeks, B. Jariwala, B. Macco, J. -W. Weber, M. van de Sanden, S. Agarwal, and C. Ciobanu  
*Carbon monoxide induced reduction and healing of graphene oxide*  
Materials Research Society Fall Meeting, Boston MA, December 2013.
  10. **B. Narayanan**, I. Reimanis, and C. Ciobanu  
*Reversible structural transition in  $\beta$ -eucryptite ( $\text{LiAlSiO}_4$ ) induced by pressure: an ab-initio metadynamics study*  
Materials Research Society Spring Meeting, San Francisco CA, April 2013.
  11. **B. Narayanan**, I. Reimanis, H. Huang, and C. Ciobanu  
*Radiation effects and tolerance mechanism in  $\beta$ -eucryptite*  
Annual Conference of Colorado Center for Advanced Ceramics, Estes Park CO, August 2012.  
**[Recipient of Best Student Presentation award]**
  12. **B. Narayanan**, A. van Duin, B. Kappes, C. Ciobanu, and I. Reimanis  
*Parameterization of the Reactive Force Field for Elastic Properties of Eucryptite Phases*  
Materials Science and Technology Conference, Houston TX, October 2010.
  13. **B. Narayanan**, A. van Duin, B. Kappes, C. Ciobanu, and I. Reimanis  
*Parameterization of the Reactive Force Field for Elastic Properties of Eucryptite Phases*  
Annual Conference of Colorado Center for Advanced Ceramics Conference, Golden CO, August 2010.  
**[Recipient of Best Student Presentation award]**
  14. **B. Narayanan**, C. Ciobanu, E. Fuller Jr., and I. Reimanis  
*Atomistic simulation of pressure induced transformation in  $\beta$ -eucryptite*  
Materials Science and Technology Conference, Pittsburgh PA, October 2009.
  15. **B. Narayanan**, S. Bhattacharya, and T. Abinandanan  
*Spinodal decomposition in epitaxial thin films*  
Indian Institute of Metals Technical Meeting, Mumbai India, November 2007  
**[Recipient of Best Oral Presentation award in the Student Symposium]**