Sesha Sai Behara

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Education

Dual Degree Program (B.Tech + M.Tech) *2014–2019*
Metallurgical and Materials Engineering (Minor – Physics)
Indian Institute of Technology Madras (IITM), Chennai, India
CGPA – **9.14** (Major CGPA – **9.38**)

Research Experience

Thermodynamic reassessment and reaction analysis of CaO-MgO system Master's thesis, *Ongoing*
Advisor: Prof. K.C. Hari Kumar, Metallurgical and Materials Engineering, IITM

- Computed ground state enthalpies of formation and mixing of CaO and MgO utilizing Vienna Ab initio Simulation Package (VASP) and Alloy Theroetic Automated Toolkit (ATAT) respectively.
- Obtained finite temperature properties such as Heat Capacity using Phonopy.
- Optimized the gibbs energy parameters for halite and liquid phases utilizing experimental data from literature and generated *ab initio* data.

Quantum Monte Carlo study of polymorphism in Boron Nitride (BN) *May – July'18*
Advisor: Dr. Kenta Hongo, Japan Advanced Institute of Science and Technology, Japan

- Computed ground state energies and determined the order of stability of hexagonal-BN, wurtzite-BN and zinc blende-BN using Quantum Monte Carlo method (QMC).
- Contrasted the results obtained with QMC technique with various other methods such as random phase approximation, van der Waals many body dispersion, etc.

***Ab initio* guided thermodynamic optimization of Fe-Ti-P system using CALPHAD method**
Advisor: Prof. K.C. Hari Kumar, Metallurgical and Materials Engineering, IITM *2018–Ongoing*

- Utilized VASP to obtain ground state enthalpies of formation of all the intermetallics involved in Fe-P, Ti-P and Fe-Ti-P systems.
- Currently optimizing the gibbs energy parameters for Fe-P, Ti-P binary systems which can further be utilized to obtain thermodynamic descriptions for the ternary Fe-Ti-P system.

Understanding the deformation behavior of as-cast high entropy alloys *2015–2016*
Advisor: Dr. Ravi Sankar Kottada, Metallurgical and Materials Engineering, IITM

- Synthesized (using arc melting) and performed mechanical (nano-indentation and compression testing) and microstructural characterization (XRD, Optical Microscopy, SEM and TEM) of CoCrFeNi, CoCrFe, CoFeNi and CrFeNi (equiatomic composition).
- Studied the influence of stacking faults on the mechanical behavior of the alloys.

Course Projects

GPU accelerated molecular dynamics simulation of solid Argon *Mar– May'17*
Advisor: Dr. Ethayaraja Mani, Chemical Engineering, IITM

- Computed the variation of thermal conductivity of solid Argon as a function of temperature using Molecular Dynamics approach.
- Computed the speed factor in GPU in comparison to a conventional CPU.

Modeling the effect of inhomogeneity on dislocations using discrete dislocation dynamics *Mar– May'18*
Advisor: Dr. Shyam Keralavarma, Aerospace Engineering, IITM

- Computed the variation of Peach Köhler force as a function of distance between inhomogenity and the dislocation dipole.
- Shear stress profiles for various configurations of inhomogeneity and the dislocation dipole were plotted and contrasted.

Conference Presentations

- **Sesha Sai Behara**, Soumya Sridar and K.C. Hari Kumar, "Gibbs Energy Description for FeTiP Precipitates in Interstitial Free High Strength (IFHS) Steels", Contributory oral presentation at National Metallurgist Day Annual Technical meet (NMD ATM) conference, Kolkata, India, November 2018.
- **Sesha Sai Behara**, Soumya Sridar and K.C. Hari Kumar, "Thermodynamic optimization of CaO-MgO system coupled with *ab initio* calculations", In house symposium, IIT Madras, India, July 2017.
- Anirudha Karati, **Sesha Sai Behara**, Amogha Skanda, Simpa Thakur, Ameey Anupam, and Ravi Sankar Kottada, "Tesseracts: Stacking faults in CoCrFe alloys", Metallography contest at National Metallurgist Day Annual Technical Meet (NMD ATM) conference, Coimbatore, India, November 2015.

Professional Experience

Industrial Internship at Rashtriya Ispat Nigam Limited, Visakhapatnam *June–July'16*

Advisor: B.Kindo, Assistant General Manager, Rashtriya Ispat Nigam Limited, Visakhapatnam, India

- Gained insights in operation and functioning of Rolling Mills, Blast Furnace and LD converter.
- Studied the effect of rolling speed on the micro-structural and mechanical properties of rebars.

Scholastic Achievements

- Awarded scholarship from Japanese Government to pursue two months research at Japan Advanced Institute of Science and Technology, Japan – 2018.
- One of the ***five*** students in the institute to be awarded Steel Scholarship offered by Ministry of Steel, Government of India – 2017.
- One of the ***100*** students of all the prestigious engineering (IITs, NITs) and management (IIMs) institutions in India to be awarded OPJEMS scholarship – 2016.
- Scored ***270/360*** in JEE Mains 2014 (Joint Entrance Examination), with only 850 students scoring above 270 out of 1.3 million applicants.
- Secured ***second*** position in All India Fast Mathematics competition – 2009.

Teaching Experience

- Teaching Assistant for **Thermodynamics and Kinetics** (MM5050) course - July – Nov 2018
- Teaching Assistant for **Metallurgical Thermodynamics** (MM2015) course - July – Nov 2017

Technical Skills

- ***Ab initio* packages**: VASP, Quantum Espresso, CASINO, ATAT
- **Other packages**: Phonopy, Thermo-Calc, LAMMPS
- **Programming Languages**: C, Python, Fortran, MATLAB, Shell scripting
- **Miscellaneous**: Auto CAD, LaTeX

Relevant Course Work

- **Physics Courses**: Quantum Physics, Classical Physics
- **Mathematics Courses**: Linear Algebra and Numerical Analysis, Differential Equations
- **Computational Courses**: Atomistic Modelling of Materials, Molecular Simulations of Soft Matter, Computational Materials Thermodynamics, Computational Fluid Dynamics, Micro Mechanics, Computational Materials Engineering
- **Basic Courses**: Materials Characterization, Metallurgical Thermodynamics, Transport Phenomena, Physics of Materials, Mechanical Behaviour of Materials, Phase Transformations

Extra-Curricular Activities

- Head of editorial team - ETCH (Department Magazine) *2016 – 2017*
- Manager of Workshops and Demonstrations team - AMALGAM (Department Festival) *2018*
- Member of Bragg group[1] – IITM *2016 – Ongoing*
- Taught underprivileged children as a part of National Service Scheme, IITM *2014 – 2015*

[1] A student group formed with the aim of learning different aspects of Computational Material Science