Dr. Sudheer Ganisetti

Materials Scientist

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About Me

Computational materials scientist with a decade of experience in glass research. Skilled in Python, C, and data analysis, with extensive expertise in scientific programming, method development, atomistic simulations, and training machine-learning force fields. Committed to integrating simulation techniques and data-driven approaches to uncover novel structure-property relationships that drive innovative materials discovery and design.

Work Experience

Aalborg University
Denmark
Dec 2022 – Present

Postdoctoral Researcher

- Generated DFT datasets and trained machine-learning force-fields (MLFF) for oxide glasses
- Studied composition-structure-property relationships using MLFF as part of the ERC-funded "NewGLASS" project

LEM3 – CNRS LAB
France
Sep 2022 – Dec 2022

Simulation Engineer

- Developed routines to use MEAM pair styles in LAMMPS to perform efficient Monte Carlo Simulations under Semi Grand Canonical Ensemble

IIT Delhi
India
Aug 2021 – Aug 2022

Research Scientist

- Successfully generated DFT data to prepare machine learning inspired force-fields for various oxide glasses
- Prepared sodium alumino-silicate glasses using computational methods & investigated structural and transport properties
- Prepared workflows for computing NMR parameters using simulations

University of Erlangen
Germany
Jan 2017 – Oct 2022

Research Associate (self – funded)

- Developed a wide array of tools in python, C, C++, bash and awk for computing & analysing several properties of glasses
- Developed novel methods for studying anisotropy in glasses
- Performed MD simulations for computing structural, mechanical, and transport properties of various glasses

University of Erlangen
Germany
Jun 2013 – Dec 2016

Research Associate

- Studied topological anisotropy of amorphous silica under the framework of 'Topological Engineering of Ultra-strong Glasses' sponsored by the German Science Foundation (DFG)
- Co-developed and implemented a polarizable potential model in the IMD software package
- Served as an administrator for a high-performance workstation dedicated to complex scientific data visualization

Ruhr University Bochum
Germany
Apr 2011 – Apr 2013

Research Assistant

- Performed DFT simulations for analysing the effects of silicon on the diffusion path of carbon in steel

SKVT Degree College
Rajahmundry, India
Sep 2008 – Mar 2009

Physics Lecturer

- Developed and delivered comprehensive lectures covering a wide range of physics topics
- Supervised laboratory experiments, ensuring students gained hands-on experience and practical skills

Programming Skills

Python | Scikit-Learn | C | MPI Parallelization | BASH Scripting | ASE | AWK Scripting | Fortran | C++ | SQL

Scientific Softwares

LAMMPS | VASP | GULP | Quantum espresso | IMD | DL_Poly | ThermoCalc | LibAtoms | OpenPhase | Abaqus | PotFit

Machine Learning FF

VASP-MLFF | DeepMD | NequIP | AllegroGraph | Allegro-Legato | MACE

Language Skills

ENGLISH– Fluent | GERMAN– A2 | TELUGU– Native

Personal Details

Date of Birth : Aug 1986
Nationality : Indian
Marital Status : Single

Education

University of Erlangen
Germany
Jun 2013 – Sep 2022

Doctor of Philosophy in Materials Science and Engineering

- Thesis: Atomistic Simulations of Silica Glass: Topological Anisotropy & Mechanical Properties
- Advisor: Prof. Erik BITZEK

Ruhr University Bochum
Germany
Mar 2011 – Apr 2013

Master of Science in Materials Science and Simulations

- Thesis: Multiscale Modelling of the Influence of Oxygen on Structure and Cohesion of ∑5 Symmetrical Tilt Grain Boundary in Molybdenum
- Advisors: Dr. Rebecca JANISCH & Prof. Alexander HARTMAIER

Pondicherry University
India
Jun 2006 – Apr 2008

Master of Science in Physics

- Thesis: Annealing of a Finite System using Montecarlo Simulations
- Advisor: Prof. Siva Kumar R

Andhra University
India
Jun 2003 – Apr 2006

Bachelor of Science in Physics

- Majors : Mathematics, Physics, Chemistry

Certifications

Data Camp
Dec 2021
Data Scientist with Python Track

Udemy
May 2021
Complete Machine Learning & Data Science Bootcamp

Udemy
May 2021
The Complete SQL Bootcamp 2021

Awards & Scholarships

University of Erlangen
Oct 2016
DAAD–STIBET Scholarship

Pondicherry University
Jun 2007
Graduate Merit Scholarship

Pondicherry University
Jun 2006
25th Rank in All India Entrance Exam

References

Prof. Morten M Smedskjaer
Full Professor
Aalborg University, Denmark
e-mail: mos@bio.aau.dk

Dr. Julien Guenole
Research Scientist
LEM3 – CNRS, Metz, France
e-mail: julien.guenole@univ-lorraine.fr

Prof. N M Anoop Krishnan
Associate Professor
Indian Institute of Technology, India
e-mail: krishnan@iitd.ac.in

Dr. Amarnath R Allu
Scientist
Glass & Ceramic Research Institute, India
e-mail: aareddy@cgcri.res.in

Web Presence

Portfolio	https://sudheerganisetti.github.io
AAU	https://vbn.aau.dk/en/persons/vnsg
LinkedIn	https://www.linkedin.com/in/sudheer-ganisetti
XING	https://www.xing.com/profile/Sudheer_Ganisetti
Github	https://github.com/sudheerganisetti
Google-scholar	https://tinyurl.com/4dx62zb2

Publications

1. **S. Ganisetti** *et al.*, "Composition-structure correlations in alkali silicate glasses based on machine-learning force fields" (*under preparation*), **2025**
2. T. Du, "Deciphering the controlling factors for phase transitions in zeolitic imidazolate frameworks" *Natl. Sci. Rev.*, vol. 11, no. 4, **2024** doi: 10.1093/nsr/nwae023
3. J . Gangareddy *et al.*, "Multi-Functional Applications of H-Glass Embedded with Stable Plasmonic Gold Nanoislands" *Small*, vol. 20, no. 1, pp. 1–18, **2024** doi: 10.1002/smll.202303688
4. S. Chakraborty *et al.*, "Enhancing glass-forming ability and mechanical properties of barium-calcium-aluminate glasses through ZnO inclusion," *J. Non. Cryst. Solids*, vol. 636, no. April, p. 123005, **2024** doi: 10.1016/j.jnoncrysol.2024.123005
5. **S. Ganisetti** *et al.*, "The origin of deformation induced topological anisotropy in silica glass" *Acta Mater.*, vol. 257, no. June, p. 119108, **2023** doi: 10.1016/j.actamat.2023.119108
6. S. R. Keshri *et al.*, "Elucidating the influence of structure and Ag+-Na+ ion-exchange on crack-resistance and ionic conductivity of Na3Al1.8Si1.65P1.8O12 glass electrolyte" *Acta Mater.*, vol. 227, p. 117745, **2022** doi: 10.1016/j.actamat.2022.117745.
7. **S. Ganisetti** *et al.*, "Ionic Conductivity of $Na_3Al_2P_3O_{12}$ Glass Electrolytes - Role of Charge Compensators" *Inorg. Chem.*, vol. 60, no. 17, pp. 12893–12905, **2021** doi: 10.1021/acs.inorgchem.1c01280. (equal contribution with R Keshri)
8. A. Gaddam *et al.*, "Effect of Vanadium Oxide on the Structure and Li-Ion Conductivity of Lithium Silicate Glasses," *J. Phys. Chem. C*, vol. 125, no. 30, pp. 16843–16857, **2021** doi: 10.1021/acs.jpcc.1c05059.
9. S. Prasad *et al.*, "Elucidating the effect of CaF_2 on structure, biocompatibility and antibacterial properties of S53P4 glass" *J. Alloys Compd.*, vol. 831, p. 154704, **2020** doi: 10.1016/j.jallcom.2020.154704
10. **S. Ganisetti** *et al.*, "Elucidating the formation of Al-NBO bonds, Al-O-Al linkages and clusters in alkaline-earth aluminosilicate glasses based on molecular dynamics simulations" *Phys. Chem. Chem. Phys.*, vol. 21, no. 43, pp. 23966–23977, **2019** doi: 10.1039/c9cp04332b.
11. A. R. Allu *et al.*, "Structure and Crystallization of Alkaline-Earth Aluminosilicate Glasses: Prevention of the Alumina-Avoidance Principle," *J. Phys. Chem. B*, vol. 122, no. 17, pp. 4737–4747, **2018** doi: 10.1021/acs.jpcb.8b01811.