Dr. Anurag Bajpai

Group Leader, Artificial Intelligence for Materials Science
Alexander von Humboldt Fellow
Max Planck Institute for Sustainable Materials, Düsseldorf, Germany
+49-15510851063 • a.bajpai@mpi-susmat.de
https://sites.google.com/view/dranuragbajpai • https://tinyurl.com/anuragbajpai

Summary of Qualifications

- Materials scientist working at the interface of physical metallurgy, autonomous materials design and sustainable metallurgy, with emphasis on bulk metallic systems, process–microstructure–property relationships, thermodynamic modeling, experimental validation and machine-guided alloy/process design.
- **Group Leader**, Artificial Intelligence for Materials Science group at the Max Planck Institute for Sustainable Materials, leading and coordinating an international multidisciplinary team of 2 Master's students, 1 PhD researcher, and 3 postdoctoral researchers working across machine learning, thermodynamics, microstructure analysis, alloy processing, and structural properties of bulk alloy systems.
- Experience developing international collaborative research proposals and PI-level materials design work packages.
- Research portfolio spans hydrogen-based reduction for green steelmaking, scrap-tolerant alloy design, multicomponent metallic glasses, high-entropy alloys, and sustainable materials processing.
- Experienced in building and leading collaborations across computational modeling, alloy processing, microscopy, thermodynamics, and data-driven materials discovery.
- Skilled in mentoring early-career researchers and integrating machine learning, physical metallurgy, microstructure analysis, and experimental validation into coherent research workflows.

Areas of Specialization

- Physical and mechanical metallurgy of bulk metallic systems
- Autonomous and physics-informed materials design
- Machine learning for microstructure-sensitive alloy design and process–microstructure–property relationships
- Sustainable metallurgy and scrap-tolerant alloy design
- Hydrogen-based reduction and green steelmaking
- Bulk metallic glasses, high-entropy and compositionally complex alloys
- Critical-material recovery and circular metallurgy

Technical Skills

Computational materials science: CALPHAD-informed thermodynamic modeling, atomistic simulation, molecular dynamics, composition–processing–property modeling, physics-informed machine learning.

Machine learning and data science: supervised and unsupervised learning, active learning, transfer learning, generative modeling, uncertainty quantification, symbolic regression, image segmentation, feature engineering, model interpretation.

Programming and software: Python, NumPy, pandas, SciPy, scikit-learn, TensorFlow/Keras, MATLAB, LAMMPS, OVITO, Origin.

Materials processing and thermal treatment: vacuum arc melting, mechanical alloying, cryomilling, pulsed laser ablation, heat-treatment design, sample preparation for microstructural (SEM and TEM) and mechanical characterization.

Characterization and microstructure analysis: high-energy synchrotron XRD, SEM, EPMA, DSC, nanoindentation, AFM, Raman spectroscopy, XPS, FTIR, UV–Vis spectroscopy, image-based microstructure quantification.

Education

Indian Institute of Technology Kanpur — **India**
M.Tech–PhD Dual Degree, GPA: 8.3/10 — *January 2017–August 2023*
Materials Science and Engineering

Ph.D. Thesis: *Compositional Design, Thermal Stability and Mechanical Behavior of Multicomponent Metallic Glasses*
M.Tech Thesis: *From Trash to Treasure - Utilization of Electronic Waste as precursors in Advanced Technologies*

Punjab Engineering College, Chandigarh — **India**
Bachelor of Engineering, GPA: 7.7/10 — *2011–2015*
Materials and Metallurgical Engineering

Professional Experience

Max Planck Institute for Sustainable Materials (formerly, MPIE) **Germany**
Group Leader, Artificial Intelligence for Materials Science
Alexander von Humboldt Postdoctoral Fellow *June 2024–present*

- Scientific host: **Prof. Dierk Raabe**
  - Lead research activities in physics-informed and uncertainty-aware machine learning for autonomous materials design, with emphasis on sustainable metallurgy, bulk metallic systems, and process–microstructure–property relationships.
  - Integrate machine learning, thermodynamic constraints, microstructure analysis, and experimental validation into coherent autonomous metallurgy workflows.
  - Scientifically coordinate research activities in the group, including technical mentoring, research planning, framework development, and research manuscript coordination.

Max Planck Institute for Iron Research (MPIE) **Germany**
Max Planck Gesellschaft Postdoctoral Fellow *March 2023–May 2024*

- Scientific host: **Prof. Dierk Raabe**
  - Developed physics-informed and interpretable machine-learning models for metallic materials design, including applications to hydrogen-based reduction, multicomponent metallic glasses, and sustainable alloy discovery.
  - Integrated thermodynamic reasoning, experimental metallurgy, atomistic insights, and data-driven modeling to study deformation, relaxation, crystallization, and process-dependent property evolution in complex metallic systems.

Tata Motors **India**
Technical Manager, Vehicle Layout Operations *September 2015–October 2016*

Selected Research Experience

Autonomous bulk materials design and process–microstructure–property modeling (MPISusMat, Present):

- Developed physics-informed and uncertainty-aware machine-learning frameworks for autonomous materials design, with applications to multicomponent metallic glasses, sustainable alloys, and hydrogen-based metallurgical processes.
- Introduced attention-enhanced variational learning for inverse design of exceptionally hard multicomponent bulk metallic glasses, combining latent-space learning, physical descriptors, and targeted property optimization.
- Developed physics-constrained constitutive learning strategies to identify rate-limiting timescales in hydrogen-based direct reduction, supporting interpretable process modeling for green steelmaking.

Scrap-tolerant structural alloys and circular metallurgy (MPISusMat, Present):

- Develop active-learning workflows for the design of high-Cu-tolerant advanced steels motivated by scrap-based alloy compositions and circular metallurgy.
- Integrate thermodynamic modeling, composition descriptors, microstructure-sensitive feature extraction, and uncertainty-aware property prediction to identify alloying strategies compatible with elevated residual impurity contents.
- Develop microscopy-based image segmentation and feature-extraction pipelines to quantify microstructural descriptors for process–microstructure–property correlation.
- Establish scrap-tolerant alloy design as a route toward sustainable structural metals with improved raw-material efficiency and reduced dependence on primary alloying resources.

Physical/mechanical metallurgy of bulk metallic glasses and compositionally complex alloys (IITK, 2017-2023):

- Developed machine-learning and thermodynamic-design strategies for multicomponent metallic glasses, including Mendeleev-number-based composition mapping and high-throughput glass-forming ability prediction.
- Combined calorimetry, nanoindentation, microstructure characterization, high-energy X-ray diffraction, deformation modeling, and molecular dynamics to study crystallization, structural relaxation, serrated flow, and time-dependent deformation in Cu–Zr-based metallic glasses.
- Established composition–structure–property relationships linking compositional complexity, free-volume sensitivity, deformation-zone connectivity, and intermittent plasticity in metallic glasses.

Sustainable metallurgy and resource recovery (IITK, 2017-2022):

- Developed cryomilling-based routes to separate and recover metallic and polymeric fractions from electronic waste for sustainable materials processing.
- Demonstrated downstream utilization of recovered components, including electrochemical CO_2 reduction, graphene synthesis from polymeric waste fractions, and rare-earth recovery using EDTA-functionalized chitosan.

Research Publications

1. **Anurag Bajpai**, Jaemin Wang, Barak Ratzker, Bilgehan Murat Sesen, Florian Kark, Dierk Raabe; *Attention-enhanced variational learning for physically informed discovery of exceptionally hard multicomponent bulk metallic glasses.* **Nature Communications**, Volume 17, 2026. DOI: 10.1038/s41467-026-73008-0. *Selected as Feature Article in Materials Science and Chemistry theme.*

2. **Anurag Bajpai**, Jaemin Wang, Barak Ratzker, Rebeca Miyar, Hendrik Holz, Nilesh P. Gurao, Krishanu Biswas, Dierk Raabe; *Coupled influence of structural relaxation and compositional complexity on deformation behavior and intermittent plasticity in Cu–Zr-based metallic glasses.* **Acta Materialia**, Volume 315, 2026. DOI: 10.1016/j.actamat.2026.122394.
3. **Anurag Bajpai**, Barak Ratzker, Pasquale Cavaliere, Dierk Raabe; *Physics-constrained constitutive learning of rate-limiting timescales for efficient hydrogen-based direct reduction for green steelmaking.* **Advanced Science**, Volume 14, 2026. DOI: 10.1002/advs.75498.
4. **Anurag Bajpai**, Jaemin Wang, Dierk Raabe; *Compositional complexity buffers free-volume sensitivity and serrated flow in metallic glasses.* **npj Computational Materials**, Volume 12, 2026. DOI: 10.1038/s41524-025-01933-7.
5. **Anurag Bajpai**, Jaemin Wang, Dierk Raabe; *Deformation zone connectivity governs time-dependent load relaxation in Cu-Zr-based metallic glasses.* **Computational Materials Science**, Volume 269, 2026. DOI: 10.1016/j.commatsci.2026.114716. *Selected as Editor's Choice Article of the Month for April 2026.*
6. Ziyuan Rao*, **Anurag Bajpai*** (*equal contribution), Hongbin Zhang; *Active learning strategies for design of sustainable alloys.* **Philosophical Transactions of the Royal Society–A**, Volume 382, 2024. DOI: 10.1098/rsta.2023.0242.
7. **Anurag Bajpai** and Krishanu Biswas; *Thermal Stability of newly developed Cu-Zr-Ag-Ti-Ni Multicomponent Bulk Metallic Glass.* **Materials Chemistry and Physics**, Volume 307, 2023. DOI: 10.1016/j.matchemphys.2023.128092.
8. **Anurag Bajpai**, Jatin Bhatt, Krishanu Biswas, and Nilesh P. Gurao; *Accelerated design of Multicomponent Metallic Glasses using Machine Learning.* **Journal of Materials Research**, Volume 37, 2022. DOI: 10.1557/s43578-022-00659-2. *Selected as Cover Article for Volume 37, Issue 15.*
9. **Anurag Bajpai**, Jatin Bhatt, Krishanu Biswas, and Nilesh P. Gurao; *A new approach to design Multicomponent Metallic Glasses using Mendeleev Number.* **Philosophical Magazine**, 2022. DOI: 10.1080/14786435.2022.2121868.
10. **Anurag Bajpai**, Partha Kumbhakar, Chandra Sekhar Tiwary, and Krishanu Biswas; *Conducting graphene synthesis from electronic waste.* **ACS Sustainable Chemistry and Engineering**, Volume 42, 2021. DOI: 10.1021/acssuschemeng.1c03817. *Selected as Cover Article for Volume 9, Number 42.*
11. Nidhi Sharma*, **Anurag Bajpai*** (*equal contribution), Chandra Sekhar Tiwary, and Krishanu Biswas; *Green Route for Beneficiation of Metallic Materials from Electronic Waste for Selective Reduction of CO_2.* **ACS Sustainable Chemistry and Engineering**, Volume 32, 2020. DOI: 10.1021/acssuschemeng.0c03605. *Selected as Cover Article for Volume 8, Number 32.*
12. **Anurag Bajpai**, Jatin Bhatt, Krishanu Biswas, and Nilesh P. Gurao; *A new perspective to thermodynamical designing of high entropy bulk metallic glasses.* **Physica B: Condensed Matter**, Volume 595, 2020. DOI: 10.1016/j.physb.2020.412350.
13. Shashank Shekhar Mishra, Khushubo Tiwari, **Anurag Bajpai**, Thakur Prasad Yadav, Ram Manohar Yadav, et al.; *Structural Evolution and Tunable Magnetic Response in novel TiZrVCrNiFe-X (X= Mn, MnCo) Alloys: An Experimental and Thermodynamic Study.* **Journal of Alloys and Compounds**, Volume 1055, 2026. DOI: 10.1016/j.jallcom.2026.186380.
14. Rahul Mitra, **Anurag Bajpai**, Krishanu Biswas; *A critical review on mechanical alloying of high-entropy materials.* **High Entropy Alloys and Materials**, Volume 3, 2025. DOI: 10.1007/s44210-025-00056-4.
15. Shruti Srivastava, **Anurag Bajpai**, and Krishanu Biswas; *Recovery of Rare Earth Elements (Nd, Dy) from spent magnets using EDTA Functionalized Chitosan.* **RSC Sustainability**, Volume 2, 2024. DOI: 10.1039/D3SU00427A.
16. Rahul Mitra, **Anurag Bajpai**, and Krishanu Biswas; *ADASYN-assisted machine learning for phase prediction of high entropy carbides.* **Computational Materials Science**, Volume 223, 2023. DOI: 10.1016/j.commatsci.2023.112142.
17. Rahul Mitra, **Anurag Bajpai**, and Krishanu Biswas; *Machine learning-based approach for phase prediction in High Entropy Borides.* **Ceramics International**, Volume 48, 2022. DOI: 10.1016/j.ceramint.2022.02.218.
18. Bejjipurapu Akhil, **Anurag Bajpai**, and Krishanu Biswas; *Microstructure and Mechanical Properties of the new TiZrHfReAl HCP High Entropy alloy.* **Philosophical Magazine Letters**, 2022. DOI: 10.1080/09500839.2022.2120644.
19. S. S. Mishra, **Anurag Bajpai**, and Krishanu Biswas; *TiVCrNiZrFex High entropy alloy: Phase evolution, Magnetic and Mechanical properties.* **Journal of Alloys and Compounds**, Volume 871, 2021. DOI: 10.1016/j.jallcom.2021.159572.
20. S. S. Mishra, **Anurag Bajpai**, and Krishanu Biswas; *Structure-Property Correlation of $Cu_2Mn_1Al_{1-x}Ga_x$ Full-Heusler Alloy.* **Journal of Alloys and Compounds**, Volume 898, 2021. DOI: 10.1016/j.jallcom.2021.162865.
21. Bejjipurapu Akhil, **Anurag Bajpai**, N. P. Gurao, and Krishanu Biswas; *Designing Hexagonal Close Packed High Entropy Alloys using Machine Learning.* **Modelling and Simulation in Materials Science and Engineering**, Volume 29, 2021. DOI: 10.1088/1361-651X/ac2b37.
22. Jitesh Kumar, Saumya Jha, Abheepsit Raturi, **Anurag Bajpai**, Reshma Sonkusare, N.P. Gurao, and Krishanu Biswas; *Novel Alloy Design Concepts Enabling Enhanced Mechanical Properties of High Entropy Alloys*. **Frontiers in Materials**, Volume 9, 2022. DOI: 10.3389/fmats.2022.868721.

Books

Anurag Bajpai, Krishanu Biswas and Arunabh Meshram, Beneficiation and Management of Technological Waste: Opportunities and Challenges, CRC Press, Taylor and Francis Group, 2025, ISBN - 9781003619680.

Patents

Anurag Bajpai, Syed Mohammad Musthaq and Krishanu Biswas; Electric Switch Casing using waste printed circuit boards (WPCBs) via Compression Molding (Published, Application No. 202411011268, 2024).

Submitted Research Proposals and Project Leadership

1. **German Principal Investigator**, Korea–Germany Joint Research Program 2026 proposal, Explainable Data-Driven Design of Impurity-Tolerant Recycled Aluminum Alloys; *submitted and under review*.
2. **Work-package Principal Investigator for AI-based materials and processing design**, Horizon Europe proposal ***CALLMA***. Responsible for AI-driven materials design concepts linking composition, processing, microstructure, and performance in sustainable alloy development; *submitted and under review*.
3. **Work-package Principal Investigator for causal-inference-based materials design**, Horizon Europe proposal ***UNI-FAST***. Responsible for developing AI-assisted causality-driven materials design workflows for sustainable alloy/process optimization and data-driven metallurgical decision-making; *submitted and under review*.

Research Leadership, Mentoring and Professional Service

- **Group Leader**, Artificial Intelligence for Materials Science group, Max Planck Institute for Sustainable Materials: lead research in physics-informed and uncertainty-aware machine learning for autonomous materials design, with emphasis on sustainable metallurgy, bulk metallic systems, and process–microstructure–property relationships.
- Coordinate a multidisciplinary team comprising 2 Master's students, 1 PhD researcher, and 3 postdoctoral researchers, with responsibilities spanning scientific mentoring, technical guidance, research planning, computational framework development, manuscript coordination, and integration of computational and experimental workflows.
- Mentored two M.Tech students during doctoral research; one mentee received the Gold Medal for Best M.Tech Thesis on machine-learning-assisted design of hexagonal close-packed high-entropy alloys.
- Developed and coordinated collaborative research activities across MPI-SusMat/MPIE, IIT Kanpur, and international partners in autonomous materials design, alloy processing, hydrogen-based reduction, metallic glasses, and sustainable metallurgy.
- Experience in setting up applied research directions connecting materials informatics, alloy processing, microstructure analysis, and structural property measurements.
- Co-organizer of the *AI-driven Materials Discovery and Design* symposium at the upcoming **MMM12**, Jeju, Korea, 8–13 November 2026.
- Guest Editor, Special Issue *Artificial Intelligence (AI) in Material Design*, *Processes* (MDPI).
- Active reviewer for **Nature Machine Intelligence**, **Communications Engineering**, **Materials Characterization**, **Journal of Alloys and Compounds**, **Advanced Engineering Materials**, **JOM** and **Transactions of the Indian Institute of Metals**.
- Teaching Assistant for Thermodynamics of Materials, Structure and Characterization of Materials, Process Engineering Laboratory, Mechanical Behavior Laboratory, and Manufacturing Processes Laboratory, at IIT Kanpur.

Conferences and Talks

Invited Talks

1: **Indian Institute of Technology (BHU) Varanasi**, titled *"Applied Materials Informatics for Alloy Design"* on 25th April 2024.

2: **Visvesvaraya National Institute of Technology (VNIT Nagpur)**, titled *"Materials Informatics for Alloy Design - Current Challenges and Opportunities"* on 21st December 2023.

3: **Indian Institute of Technology (IIT) Indore**, titled *"Material Informatics based High Entropy Alloy Design"* on 24th November 2023.

4: **Indian Institute of Technology (IIT) Kanpur**, organized by Materials Advantage IIT Kanpur Chapter, titled *"Machine Learning in Materials Science"* on 28th September 2023.

Oral/Poster Presentations

5: Poster Presentation at **Ab initio Description of Iron and Steel (ADIS2023)** organized by Max Planck Society at Rinberg Castle, Tegernsee from 29th October to 3rd November 2023.

6: Poster Presentation at **5th Materials Chain International Conference – MCIC 2023** organized by Ruhr-Universität Bochum, Germany on August 31, 2023.

7: Poster Presentation at **Research Scholars' Day 2022 (Padarth)** organized by the Department of Materials Science and Engineering, IIT Kanpur on 7th May 2022 (Received **Best Poster Award**).

8: Oral Presentation at **Research Scholars' Day 2022 (Padarth)** organized by the Department of Materials Science and Engineering, IIT Kanpur on 7th May 2022.

9: Oral Presentation at **Scientific Research Convention 2022** organized by IIT Kanpur and IEEE from 4th to 6th March 2022 (Received **Best Oral Presentation Award**).

10: Poster Presentation at **TMS 2022 Annual Meeting** organized by the American Institute of Mining, Metallurgical, and Petroleum Engineers (AIME) from 3rd to 7th March 2022.

11: Poster Presentation at **Indian Institute of Metals - Annual Technical Meeting (IIM-ATM) 2021** organized by the Indian Institute of Metals and Tata Steel from 13th to 15th November 2021 (Received **Two Best Poster Awards**).

Recognition and Awards

Honours and Fellowships

2024: Appointed Group Leader for the **Artificial Intelligence in Materials Science** at the Max Planck Institute for Sustainable Materials (Formerly Max Planck Institute for Iron Research, MPIE, GmbH), Germany.

2024: Awarded the **Alexander von Humboldt Postdoctoral Fellowship** for research at the Max Planck Institute for Sustainable Materials (Formerly Max Planck Institute for Iron Research, MPIE, GmbH), Germany.

2023: Awarded **Research Fellowship** by the **Max-Planck-Gesellschaft** (**Max Planck Society**) for postdoctoral research at the Max Planck Institute for Iron Research, MPIE, GmbH, Germany.

2016: Recipient of the **MHRD Fellowship** provided by the Government of India to pursue master's and doctoral research.

Awards

2026: Article titled *"Attention-enhanced variational learning for physically informed discovery of exceptionally hard multicomponent bulk metallic glasses"* selected for the **Nature Communications Editors' Highlights** under the **Materials science and chemistry** theme.

2026: Article titled *"Deformation zone connectivity governs time-dependent load relaxation in Cu-Zr-based metallic glasses"* selected as **Editor's Choice Article of the Month** for April 2026 of the journal **Computational Materials Science**.

2022: Article titled *"Accelerated Design of Multicomponent Metallic Glasses using Machine Learning"* selected as **Journal Cover** for Volume 37, Issue 15 of the **Journal of Materials Research**.

2022: **Best Poster Award** on Research Scholars' Day 2022 organized by the Department of Materials Science and Engineering, IIT Kanpur, India.

2022: **Best Oral Presentation Award** at Scientific Research Convention 2022 organized by the Indian Institute of Technology Kanpur and IEEE.

2021: Article titled *"Conducting Graphene Synthesis from Electronic Waste"* featured as **Journal Cover** for Volume 9, Number 42 of **ACS Sustainable Chemistry and Engineering**.

2021: Won **Two Best Poster Awards** under the *Energy-Environment & Waste Utilization* and *Advances in Material Science & Technology* themes at the **Indian Institute of Metals 75th Annual Technical Meeting**.

2020: Article titled *"A Green Route for Beneficiation of Metallic Materials from Electronic Waste for Selective Reduction of CO_2"* featured as **Journal Cover** for Volume 8, Number 32 of **ACS Sustainable Chemistry and Engineering**.

References

1: **Prof. Dierk Raabe**,
Director, Max Planck Institute for Sustainable Materials, Düsseldorf, Germany.
Email: d.raabe@mpi-susmat.de.
Phone: (+49) (211) 6792 278.

2: **Prof. Krishanu Biswas**,
Department of Materials Science and Engineering, Indian Institute of Technology Kanpur, India.
Email: kbiswas@iitk.ac.in.
Phone: (+91) (512) 259 6184.

3: **Prof. Nilesh P. Gurao**,
Department of Materials Science and Engineering, Indian Institute of Technology Kanpur, India.
Email: npgurao@iitk.ac.in.
Phone: (+91) (512) 259 6688.