Dr. Snehanshu Pal

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Website : https://www.iiests.ac.in/IIEST/Faculty/metal-snehanshu
Web of Science Profile : https://www.webofscience.com/wos/author/record/D-2082-2012
Google Scholar Profile: https://scholar.google.co.in/citations?user=1asrimkAAAAJ&hl=en
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Profile Summary

Research Areas:	Computational Materials Engineering, Extractive Metallurgy, Metallurgical Process Modeling, Materials Informatics.
Research Profile Keywords:	Atomistic Simulations, Machine Learning, Steel Making Process, Molecular Dynamics Simulation, Density Functional Theory, Grain Boundary Engineering.
Books Published as author:	Three (3)
Book Published as editor:	One (1)
SCI journal Article Published:	One hundred twenty four (124)
Doctoral Students Supervised:	Eleven (11)
Master Students (M. Tech) Supervised:	Sixteen (16)
Sponsor Research Projects:	Seven (7)
Consultancy Research Project:	Three (3)
Research/Teaching Experience:	More than Twelve (12) years
Industrial Experience (Steel Industry):	More than Three (3) Years

Education

2009-2013 | Ph.D. Metallurgical and Materials Engineering,
Indian Institute of Technology, Kharagpur, India
Research Topic: Atomistic Simulations of Methane Hydrates and Inhibitor Design

1998-2002 | B.E. Metallurgical and Materials Engineering, First Division,
Bengal Engineering college (Deemed University), Shibpore, Howrah, India (currently known as **Indian Institute of Engineering Science and Technology,** Shibpur Howrah, India).

Research /Academic Experience

Sept.2023- Present	Associate Professor, Department of Metallurgy and Materials Engineering, **Indian Institute of Engineering Science and Technology**, Shibpur-711103,India **Research Area:** Computational Materials Engineering, Material Informatics, Process Modeling
Mar.2023- Sept.2023	Associate Professor, Department of Metallurgical and Materials Engineering, **National Institute Of Technology**, Rourkela-769008,India **Research Area:** Computational Materials Engineering, Material Informatics, Process Modeling
Feb.2014- Mar.2023	Assistant Professor, Department of Metallurgical and Materials Engineering, **National Institute Of Technology**, Rourkela-769008,India **Research Area:** Computational Materials Engineering, Material Informatics, Process Modeling
Sept.2013- Feb.2014	Post-Doctoral Fellow, **Materials Science and Engineering, the Pennsylvania State University,** United States of America(USA) **Research Area:** Computer modeling of heat transfer, material flow in welding process

Industrial Experience

Mar 2006 - July 2009	Organization: **Steel Authority of India Limited, Government of India, India** Department: **Steel Melting Shop of Rourkela Steel Plant, Rourkela, Odisha, India** Designation: **Junior Manager (Operation) – Shift in-charge**

Research Investigator of Sponsored Projects

Principal Investigator

1. **Investigation of solidification process and prediction of microstructure during secondary cooling in continuous casting of plain carbon steel to estimate the porosity fraction and carbon segregated by multi scale simulation (cellular automata and phase field modeling techniques).**
Funding Agency: Department of Science and Technology (DST), Government of India, State Committee on Science and Technology, Belarus.
Total Project Value: INR 8.83 lakhs
Present Status: Completed

2. **The effect of shock wave, moisture and sea water on debonding of multilayer in FRP composite systems -Experimental and multi-scale modeling based investigation**
Funding Agency: Naval Research Board (NRB), DRDO, Government of India
Total Project Value: INR 19.932 lakhs
Present Status: Completed

3. **Investigation of atomistic structural evolution of water/aquatic ethanol medium in the presence of homeopathy medicine substance considering the physico-chemico-mechno influences**
Funding Agency: Central Council for Research in Homoeopathy (An Autonomous Body of Ministry of Ayush), Government of India
Total Project Value: INR 40.2508 lakhs
Present Status: Ongoing

4. **ICME-enabled high-throughput experimentation and mechanical testing for developing next-generation alloys for aerospace applications**
Funding Agency: Anusandhan National Research Foundation, the Department of Science and Technology (DST), Government of India
Total Project Value: INR 474.95 lakhs
Present Status: Ongoing

Research Investigator of Sponsored Project

Co-Principal Investigator	5. **Digitization of steel microstructure images, modelling of plain carbon steel microstructure evolution during heat treatment using cellular automata and phase field modeling methods, and development of a software tool for providing guidance in designing heat treatment process using machine learning based classification techniques** **Funding Agency:** Department of Science and Technology, Government of India **Total Project Value:** INR 18.546 lakhs **Present Status:** Completed 6. **Characterization and numerical simulation of brazed joint - ceramic ring of HVB (High Voltage Bushing)** **Funding Agency:**Board of Research in Fusion Science and Technology (BRFST), BRNS, Government of India **Total Project Value:** INR 25.64 lakhs **Present Status:** Completed 7. **Failure analysis and Cost estimation for AC submerged arc furnace.** **Funding Agency:**SARAF Agencies pvt. ltd. **Total Project Value:** INR 3.00 lakhs **Present Status:** Completed

Research Investigator of Consultancy Project

Principal Investigator	1. **Optimizing minor constituents in blast furnace slag to operate 19-22 percentage slag Alumina** **Funding Agency:** Tata Steel Ltd. **Total Project Value:** INR 19.90 lakhs **Present Status:** Completed
Principal Investigator	2. **Investigation on Hydrogen Diffusion in High Entropy Alloy** **Funding Agency:** CSIR- Indian Institute of Petroleum **Total Project Value:** INR 3.00 lakhs **Present Status:** Completed
Principal Investigator	3. **Investigation for premature breakage of Lock in Centre Buffer Coupler as used in Indian Railway Freight Wagons,** **Funding Agency:** Lalbaba Engineering Group 27, Shakespeare Sarani, Kolkata - 700017, West Bengal, India, **Total Project Value:** INR 1.23 lakhs **Present Status:** Completed

Achievements

1. Indian Institute of Metal (IIM) - Steel Authority of India Limited (SAIL) Gold Medal (Ferrous Category), 2024

2. Ranked 30th (all India rank) in Graduate Aptitude Test in Engineering (GATE) 2009

Courses Taught as Course Teacher

At National Institute of Rourkela, India

Subject No.	Subject Name	L-T-P
MM611	Process Modelling for Steel Industry	3-0-0
MM6311	Metallurgical Thermodynamics and Kinetics	3-0-0
MM2302	Transport Phenomenon	3-0-0
MM472	Thermodynamic Modeling of Metallic systems	0-0-3
MM305	Steel Making	3-0-0
MM426	Secondary Steel Making	3-0-0
MM274	Atomistic Modeling of Materials Laboratory	0-0-3
MM476	Computational Modeling of Process Metallurgy Laboratory	0-0-3
MM494	Seminar and Technical Writing – II	0-0-0

At Indian Institute of Engineering Science and Technology Shibpur, India

Subject No.	Subject Name	L-T-P
MM3223N	Computational Materials Engineering	3-0-0
MM5203N	Multiscale Materials Modelling	3-0-0
MM3215	Alloy Steels and Cast Irons	4-0-0
MM2209	Iron Making	3-0-0
MM3110	Steel Making	3-0-0
MM3223N	Computational Materials Engineering Laboratory	0-0-3

Supervised Ph.D. Thesis Works as A single/sole supervisor (Total No. 4)

Sl.No.	Degree and year	Title of Thesis	Name of the Student
1.	Ph.D. (2019) Degree awarded	Molecular Dynamics Simulation Based Study for Creep Deformation Behaviour of Nanocrystalline Nickel and Nickel-Zirconium Alloys (**Obtained Institute Gold Medal for the best Ph.D.Thesis of 2019-20 in National Institute of Technology Rourkela , India**)	Dr. Md. Meraj
2.	Ph.D. (2021) Degree awarded	Molecular Dynamics Simulation Of Deformation Behaviour During Nanoscale Rolling	Dr. K. Vijay Reddy
3.	Ph.D. (2023) Degree awarded	Molecular dynamics simulation of deformation behavior of Al90Sm10 metallic glass and Al-Al90Sm10 crystalline-amorphous nanolaminate	Dr. S. Mishra
4.	Ph.D. (2024) Degree awarded	Study of radiation damage in metallic systems using molecular dynamics simulations nanolaminate	Dr. M. Manna

Supervised Ph.D. Thesis Works as A Principal supervisor (Total No. 2)

Sl.No.	Degree and year	Title of Thesis	Name of the Student
5.	Ph.D. (2023) Degree awarded	Molecular dynamics simulation of deformation Behavior of nanocrystalline Al and CNT reinforced nanocrystalline Al nanocomposites	Dr. P N Babu
6.	Ph.D. (2023) Degree awarded	The effect of shock wave, moisture and sea water on de-bonding of multilayer in FRP composite systems experimental and multi-scale modeling based investigation	Dr. S. Gupta

Supervised Ph.D. Thesis Works as A joint supervisor (Total No. 5)

Sl.No	Degree and year	Title of Thesis	Name of the Student
7.	Ph.D. (2018) Degree awarded	Fabrication of Nano-Y2O3 Dispersed Tungsten Alloys by Mechanical Alloying Followed by Conventional and Spark Plasma Sintering	Dr. A. Patra
8.	Ph.D. (2020) Degree awarded	Laser weld-brazing of aluminum alloy (AA6082/AA5083) and galvanized interstitial free steel with an emphasis on fatigue and corrosion study	Dr. N. Chary
9.	Ph.D. (2021) Degree awarded	Investigation of Deformation Behavior of High Entropy Alloy Coated FCC Metallic Systems under Nanoindentation using Molecular Dynamics Simulation	Dr. D. Mishra
10.	Ph.D. (2022) Degree awarded	Refinement and Processing of Steel Microstructure Images Facilitating Automated Heat Treatment Process Prediction	Dr. A Panda
11.	Ph.D. (2024) Degree awarded	Design of Oxygen Donor Ligands for Selective Separation of Lanthanides	Dr. A. Pati

Supervised M. Tech Thesis Works (Total No. 16)

Sl. No.	Degree and year	Title of Thesis	Name of the Students
1.	M.Tech (2023)	Optimizing minor constituents in blast slag to operate 19-22 percentage slag Alumina using material informatics approach	Mr. Devi Dutta Biswajeet
2.	M.Tech (2022)	Evaluation of structural properties and thermoelectric properties of quaternary oxides.	Mr. Ginnarapu Shivakrishna
3.	M.Tech (2022)	Investigation of molecular interaction of protein with hydroxyapatite surface using atomistic scale computational modelling technique.	Mr. Saurav Singh
4.	M.Tech (2022)	Molecular Dynamic Simulation of Mechanical Behaviour of Magnesium during Nano-indentation and Ballistic Penetration	Mr. Pragyan Goswami
5.	M.Tech (2020)	Molecular Dynamic Simulation of Nano Scale Friction Stir Welding	Mr. Roshan Kumar Jha
6.	M.Tech (2019)	Modelling of trajectory of steel droplet and determination of residence time in slag during steel refining process using CFD	Mr. Prabhash Kumar
7.	M.Tech (2018)	Modeling of solidification process and estimation of carbon segregation occurred during secondary cooling stage of continuous casting process of plain carbon steel	Mr. Gaddam Vishal
8.	M.Tech (2018)	Optimization of Ferrochrome Addition Using Multi-Objective Evolutionary and Genetic Algorithms for Stainless Steel Making via AOD Converter	Mr.Kishore Kumar Behera
9.	M.Tech (2017)	Mechanical performance evaluation of woven and unidirectional GFRP composite through numerical simulation	Mr. Yogesh Shamsundar Mhetre
10.	M.Tech (2017)	Finite Element Analysis for adhesive bonding strength of steel and FRP composite joint	Mr. Bansal Darji VinayKumar
11.	M.Tech (2016)	The Influence of Chromium Amount, Casting Speed and Superheat on The Columnar to Equiaxed Transition and Metallurgical Length for Continuously Cast Ferritic Stainless Steels	Mr. Ritesh Padhi
12.	M.Tech (2016)	Dynamic process modeling of stainless steel making through AOD converter	Mr. Jagdish Nayak
13.	M.Tech (2016)	Prediction of microstructure for heat treatment process in dual phase steels using Cellular Automata	Mr. Vijay Reddy
14.	M.Tech (2016)	Numerical Study of Post Welds Residual Stress and Creep Behavior of Inconel 718 and 316 Stainless Steel Joints	Mr. Bhardwaj Ravindra Giriraj
15.	M.Tech (2015)	Computational Fluid Dynamic (CFD) simulation for continuous casting process of steels	Mr. RahulKumar
16.	M.Tech (2015)	Mathematical Modelling of Basic Oxygen Steel Making Process	Miss Vinita Kumari

Supervised B. Tech Thesis Works (Total No. 21)

Sl. No.	Degree and year	Title of Thesis	Name of the Students
1.	B.Tech (2023)	Financial Spectrum of Boeing 737 and its Dependence on Component-wise Material Selection.	Aayush Dinesh Kandpal
2.	B.Tech (2023)	A Molecular Dynamics Study of Shock Induced Viscosity of Fe-Cr Alloys using Green Kubo relation and its Dependence on Temperature.	Shantanu Khawas
3.	B.Tech (2023)	Machine learning based phase prediction model for multi-principal element alloys and web based application development.	Neeraj Kumar
4.	B.Tech (2023)	Interfacial diffusion behaviour bimetallic system.	Sudeeksha Vandrangi
5.	B.Tech (2022)	Dynamic assessment of grain boundary, solute and dislocation interaction in FCC metal	Tapashree Pradhan
6.	B.Tech (2022)	Effect of Grain Boundary and Interficial Energy Anisotropy on Ternary Phase Separation	Abhinav Roy
7.	B.Tech (2021)	Simplementation of machine Learning for coordinating among process variable, composition and turn down Temperature for Basic Oxygen Steel making process.	Suraj Hansdah
8.	B.Tech (2021)	Study of Dislocation Precipitate Interaction in Ni-Al System Through Molecular Dynamic Simulation.	Nichenametla Jai Sai
9.	B.Tech (2021)	Ab-initio prediction and analysis of novel d0 Heusler alloys.	Adesh Rohan Mishra
10.	B.Tech (2021)	Molecular Dynamics simulation-based study on the shock response of Ni bicrystals	Tanmay Konnur
11.	B.Tech (2020)	Study of Fluid Flow Behaviour in Secondary Steel making using computational fluid dynamics	Dibya Ranjan Sahoo
12.	B.Tech (2019)	Study of creep behavior of Ni62Nb38 metallic glass	B Anjali
13.	B.Tech (2019)	Creep-ratcheting interaction study of nanocrystalline nickel using atomistic simulation	Sushrita Dash
14.	B.Tech (2019)	Evolution of dislocation density in the Ni(metal) -NiTi(metallic glass) interface with the variation in interfacial area and size of the sample	Priyansha Nikita
15.	B.Tech (2018)	Influence of Dislocation density and grain size on precipitation kinetics in P92 grade steel	Karanam Gururaj
16.	B.Tech (2018)	Influence of specimen size and strain rate on tensile deformation and fracture behavior of single-layer Silicene	B.S.K. Gargeya

Supervised B. Tech Thesis Works (Total No. 21) continued..

Sl. No.	Degree and year	Title of Thesis	Name of the Students
17.	B.Tech (2017)	Attempt to identify strategy for micro structure modelling of low carbon steel	Mr.Ankit Surana
18.	B.Tech (2017)	The influence of void and porosity on deformation behaviour of nanocrystalline Ni under tensile followed by compressive loading	Mr.Kumar Krishanjeet
19.	B.Tech (2017)	Microstructure prediction during Inter Critical Heating and Subsequent Cooling of Low Carbon Steel	Mr.Ayush Poddar
20.	B.Tech (2016)	Process For Extraction of Titanium Oxide From Ilmenite Ore by Application of Coke	Mr.Anurag Mishra
21.	B.Tech (2015)	Density Functional Theory Based Investigation of 1- Butyl-3-Methylidazolium as a Potential Methane Hydrate Inhibitor	Mr.Satyam Choudhury

Referee or Reviewer for the Journals

1. Computational Material Science
2. Steel Research International
3. Acta Materilia
4. Journal of Materials Engineering and Performance
5. Intermetallics
6. Engineering Computation
7. Journal of Materials Science and Technology
8. Materials Chemistry and Physics
9. International Journal of Mechanical Sciences
10. Journal of Alloys and Compounds
11. Journal of Material Research and Technology
12. Nature Communications
13. Modelling and Simulation in Materials Science and Engineering
14. Machine Learning: Science and Technology
15. Journal of Nanostructure in Chemistry
16. Indian Institute of Metals Transactions
17. Journal of Molecular Modeling
18. Materials Letters
19. Journal of Physics: Condensed Matter
20. Journal of Applied Physics
21. Sadhana
22. Emergent Materials
23. International Journal of Energy Research
24. Journal of Non-crystalline Solids
25. Mechanics of Materials
26. Advances and Applications in Bioinformatics
27. Computational Condensed Matter
28. Engineering Failure Analysis

29. Journal of Materials Research
30. Signal Processing: Image Communication
31. Journal of Institute of Engineers(India): Series C
32. Materials & Design
33. Applied Physics A
34. The European Physical Journal B
35. Chemical Engineering Science
36. Journal of Computational Design and Engineering
37. Journal of Materials Science
38. Physica Scripta
38. Iron Making and Steel making

Invited Talk/Lecture

1. Lecture on "Industry 4.0 – Smart Manufacturing Integration in Welding" by **Snehanshu Pal (Invited Speaker)**in the short term course program titled ""Welding of Metallic Systems and Industry 4.0: Bridging Fundamentals with Smart Manufacturing" held on 6-7 November 2025 organized by Indian Institute of Metals (India)

2. Lecture on "Physical Metallurgy of Welding – Part I (Ferrous Metals)" by **Snehanshu Pal (Invited Speaker)**in the short term course program titled ""Welding of Metallic Systems and Industry 4.0: Bridging Fundamentals with Smart Manufacturing" held on 6-7 November 2025 organized by Indian Institute of Metals (India)

3. Lecture on "Fundamentals of Machine Learning: Industrial Perspective" by **Snehanshu Pal (Invited Speaker)**in the short term course program titled "Machine Learning and Industrial Process Metallurgy" held on 8-10 January 2025 organized by Indian Institute of Metals (India)

4. Themed Tech Talk on "Scope of Interdisciplinary Research" by **Snehanshu Pal (Invited Speaker)** on December 17th 2018 organised by Intelligent Systems Research Group, School of Computer Science, UPES, Dehradun (India)

5. Lecture on "Advancement in Steel Making: Industrial Prospective" by **Snehanshu Pal (Invited Speaker)** on October 1st 2018 in the workshop titled "Advancement in Iron and Steel Making: Industrial Prospective" organised by Department of Metallurgical and Materials Engineering, OPJU, Raigarh (India)

6. Talk on "Quality Assessment through Information and Modeling for Composite Materials" by **Snehanshu Pal (Invited Speaker)** on Workshop 17th- 18th May 2018 organised by Tata Steel, Jamshedpur (India)

7. "Creep Behaviour Study of Nano-crystalline Stainless Steel and Nano-crystalline Nickel Join Using Molecular Dynamics Simulation" By Md. Meraj and **Snehanshu Pal (Keynote Speaker and Corresponding Author)**, 4th International Conference on Thermo-mechanical Simulation and Processing of Steels (Simpro'2016), February 10th- 12th 2016, RDCIS, SAIL, Ranchi (India)

8. Lecture on "Application of Computational Materials Engineering on Materials Characterization and Property Evaluation" by **Snehanshu Pal (Invited Speaker)** in Technical Education Quality Improvement Programme (TEQIP-II) sponsored Workshop on "Advanced Techniques in Materials Characterization" on 22nd- 23rd January 2016 organized Department of Metallurgical Engineering, NIT Raipur

Book Published as author (Total No. 3)

3. "Molecular Dynamics for Materials Modeling: A Practical Approach using LAMMPS Platform", **Snehanshu Pal**, K. Vijay Reddy ISBN: 9781032347196 , CRC Press, Boca Raton, USA, **2024**.

2. "Molecular Dynamics Simulation of Nanostructured Materials An Understanding of Mechanical Behavior", **Snehanshu Pal**, Bankim Chandra Ray, ISBN: 9780367029821, CRC Press, Boca Raton, USA, **2020**.

1. "Process Modeling for Steel Industry", **Snehanshu Pal**, Anshuman Patra, Prabodh Ranjan Padhee, ISBN : 9789385909399, I.K. International Publishing House Pvt. Ltd, India, **2018**.

Book Published as editor(Total No. 1)

1. "Processing and Characterization of Materials", **Dr.Snehanshu Pal**, Dr. Debdas Roy, Dr. Sudip Kumar Sinha, ISBN: 9789811639364,Springer Nature, Singapore Pte Ltd.,**2021**.

Published Book Chapter

1. Book chapter title "Dynamic Structural Evolution of Nanocrystalline Aluminum During Ratcheting Deformation" by P. Narendra Babu, K. V. Reddy and **Snehanshu Pal** of the Book, titled "Nano Scaled Structural Problems: Static and Dynamic Behaviors", Chapter no. 6 , ISBN: 9780735422865006, AIP Publishing (2021).

2. Book chapter title "Creep Behaviour Study of Nano-crystalline Stainless Steel and Nanocrystalline Nickel Join Using Molecular Dynamics Simulation" by Md. Meraj and **Snehanshu Pal** of the Book, titled "Thermo-Mechanical Simulation and Processing of Steels", Chapter no. 14 , ISBN: 978-93-85919-86-2, Viva Books Private Limited (2016).

3. Book chapter title "CFD Modeling of Fluid Flow Behavior and Bath Surface Deformation in LD Converter" by T. K. Kundu and **Snehanshu Pal** of the Book, titled "CFD Modeling and Simulation in Materials Processing", Chapter no. 38 , ISBN: 978-1-1182-9615-8 , Wiley online library (2012).

SCI Journal Article Publications (Total No. 124)

2025:

124. " Effect of welding time on the mass diffusivity and interfacial corrosion behavior of diffusion-welded joint of SDSS|NiA|Zr702", A. Kumar,S. Mukhopadhyay, **S. Pal** , S. Kundu,**Welding in the World** (2025). DOI: https://doi.org/10.1007/s40194-025-02246-5

123. " Deformation Behavior Study of Single Crystal BaPt2 Compound Using Parameterized Embedded-Atom Method Potential: Part 2—Ratcheting Characteristics", S. Mukhopadhyay, S. K. Dinda, S. K. Singh, M. Ghosh, **S. Pal** , **Journal of Engineering Materials and Technology** (2025). DOI: https://doi.org/10.1115/1.4070120

122. " Deformation Behavior Study of Single Crystal BaPt2 Compound Using Parameterized Embedded-Atom Method Potential—Part 1: Tensile and Creep Characteristics", S. Mukhopadhyay, S. K. Dinda, S. K. Singh, M. Ghosh, **S. Pal** , **Journal of Engineering Materials and Technology** (2025). DOI:https://doi.org/10.1115/1.4070121

121. " Development of a force-matched embedded-atom method (EAM) potential for rhodium-barium alloy system", S. Mukhopadhyay, S. K. Dinda, **S. Pal (Corresponding Author)**, **Journal of Engineering Materials and Technology** (2025). Philosophical Magazine, DOI: https://doi.org/10.1080/14786435.2025.2570919

120. " Molecular Dynamics Simulation Study of Irradiated High-Entropy Alloy with Crystalline–Amorphous Nanolaminate", M. Manna, S. K. Singh , **S. Pal (Corresponding Author)**, **High Entropy Alloys Materials** (2025). DOI: https://doi.org/10.1007/s44210-025-00059-1

119. " Role of grain architecture in shock behavior and spalling behavior of Al metal-Al90Sm10 metallic glass nanolaminates. ",S. Mishra, , K. Vijay Reddy, **S. Pal (Corresponding Author)**, **Shock Waves 35, 361–380** (2025). DOI: https://doi.org/10.1007/s00193-025-01231-7

118. "Effect of structural modulation of B2 phase on the deformation mechanism in FeNi-CrCoAl high entropy alloy: an atomistic insight", K. Vijay Reddy, P. Kumar, S. Vashistha, , **S. Pal** , S. K. Singh,**Materials Chemistry and Physics** (2025).
DOI: https://doi.org/10.1016/j.matchemphys.2025.130840.

117. "Developing new high-entropy alloys with enhanced hardness using a hybrid machine learning approach: integrating interpretability and NSGA-II optimization",D. Dey, A. Pal, P. Biyani, P. Mandal,**S. Pal** , S. Das, S. Dey , M. Ghosh **Journal of Materials Science 60, 4820–4845** (2025). DOI: https://doi.org/10.1007/s10853-025-10729-5

2024:

116. " Irradiation Damage Evolution Dependence on Misorientation Angle for Sigma 5 Grain Boundary of Nb: An Atomistic Simulation-Based Study", M. Manna, **S. Pal (Corresponding Author)**, **Journal of Engineering Materials and Technology** (2024).
DOI:https://doi.org/10.1115/1.4067132

115. " Predicting viscosity for steelmaking slag: A stacking regression approach", M. K. Singh, K. K. Singh, , **S. Pal (Corresponding Author)**, **Ironmaking Steelmaking: Processes, Products and Applications** (2024). DOI:https://doi.org/10.1177/030192332412658

114. " Development of embedded-atom method (EAM) potential for Palladium–Barium alloy",, **S. Pal (Corresponding Author)**, S. Mukhopadhyay, **Molecular Simulation, 50(14), 991–1000** (2024). DOI:https://doi.org/10.1080/08927022.2024.2376327

113. "Inter-property Correlation of Al2O3-CaO-MgO-SiO2 Quaternary Slag System in Blast Furnace Ironmaking",S. Hazra, D. D. Biswajeet,**S. Pal** , S. Sengupta, S. Nag , S. Seetharaman, **Journal of Phase Equilibria and Diffusion** (2024). DOI: https://doi.org/10.1007/s11669-024-01123-w

112. "Exploring the influence of bis-phosphine ligands on lanthanide complexes: A DFT study",A. Pati, T.K. Kundu,**S. Pal** , **Computational and Theoretical Chemistry** (2024). DOI: https://doi.org/10.1016/j.comptc.2024.114568

111. "Chelating effect of alizarin-oxalate on La3+ and Nd3+ in acidic, basic and neutral medium: a DFT study",A. Pati, T.K. Kundu,**S. Pal** , **Theoretical Chemistry Accounts** (2024). DOI: https://doi.org/10.1007/s00214-024-03094-0

110. "Molecular dynamics simulations of tensile and creep-ratcheting behaviour of CNT reinforced columnar nanocrystalline Al nanocomposites",D. D. Biswajeet,P. N. Babu **S. Pal (Corresponding Author)**, **Diamond and Related Materials** (2024).
DOI: https://doi.org/10.1016/j.diamond.2024.110850

2023:

109. "Residual stress and creep strain analysis of Inconel 718 and stainless steel 316 welds",R. G. Bhardwaj **S. Pal** , **Welding in the World** (2023). DOI: https://doi.org/10.1007/s40194-023-01648-7

108. " Atomistic simulation of rolling contact fatigue behavior of a face-centered cubic material (nickel)", P. Goswami, **S. Pal (Corresponding Author)**, M. Gupta,**Fatigue and Fracture of Engineering Materials and Structures** (2023). DOI: https://doi.org/10.1111/ffe.14196

107. " Investigation on wear-resistance of nanocrystalline Pt-Au by molecular dynamics simulations", T. Pradhan, **S. Pal (Corresponding Author)**, C. Deng,**Tribology International** Vol. 189, pp. 108966 (2023). DOI: https://doi.org/10.1016/j.triboint.2023.108966

106. " A molecular dynamic simulation-based study on nanoscale friction stir welding between copper and aluminium", R. K. Jha, K. V. Reddy, **S. Pal**, **Molecular Simulation**, pp. 1-12 (2023). DOI: https://doi.org/10.1080/08927022.2023.2279135

105. " Correlation and Prediction of Molten Steel Temperature in Steel Melting Shop Using Reliable Machine Learning (RML) Approach ", M. K. Singh, A. Choudhury, D. Uikey, **S. Pal**,**Transaction of the Indian Institute of Metals** Vol. 76, pp. 3365–3377 (2023). DOI: https://doi.org/10.1007/s12666-023-03005-0

104. " Unveiling the effect of interface on torsional behavior of crystalline Al-Al90Sm10 metallic glass nanolaminates ", S. Mishra, **S. Pal (Corresponding Author)**, **Philosophical Magazine** Vol. 103, pp. 1-24 (2023). DOI: https://doi.org/10.1080/14786435.2023.2219463

103. " Optimization of high alumina slag practice in blast furnace ironmaking: an industrial approach. Part 2: Data-driven aspects ", **S. Pal**, M. Sahoo, D.D. Biswajeet, S. Hazra, G.S. Tarachand, D. Bhattacharyya, S. Nag, S. Seetharaman, **Journal of Ironmaking and Steelmaking** Vol. 50, pp. 1-14 (2023). DOI: https://doi.org/10.1080/03019233.2023.2210903

102. " Optimization of high alumina slag practice in blast furnace ironmaking: an industrial approach (PART 1: fundamental aspects) ", S. Hazra, **S. Pal**, D.D. Biswajeet, M. Sahoo, G.S. Tarachand, D. Bhattacharyya, S. Nag, S. Seetharaman, **Journal of Ironmaking and Steelmaking** Vol. 50, pp. 1-14 (2023). DOI: https://doi.org/10.1080/03019233.2023.2210901

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13. ”Molecular Dynamics based Cohesive Zone Modelling of Al(metal)-Cu50Zr50 (metallic glass)interfacial mechanical behaviour and investigation of dissipative mechanism”, Pradeep Gupta, **S Pal** and N. Yedla, **Materials and Design**, Vol. 105, pp. 41- 50 (2016). DOI: https://doi.org/10.1016/j.matdes.2016.05.054

12. “Optimization of phosphorous in steel produced by basic oxygen steel making process using multi-objective evolutionary and genetic algorithms”, **S Pal (Corresponding Author)**, C. Halder, **Steel Research International**, Vol. 88(3), pp. 1600193 (2016). DOI: https://doi.org/10.1002/srin.201600193

11. ”Role of W on the Deformation behaviour of Ni-W Alloy under Tensile Followed by Compressive Loading” M Meraj, N. Yedla, **S Pal (Corresponding Author)**, **Metals and Materials International**, Vol.22 (3),pp. 373-382(2016). DOI:https://doi.org/10.1007/s12540-016-5551-6

10. “The Effect of Temperature on Creep Behaviour of Porous (1 at.percent) Nano Crystalline Nickel”. M. Meraj and **S Pal (Corresponding Author)**, **Transactions of the Indian Institute of Metals**, Vol. 69, pp. 277-282 (2016). DOI:https://doi.org/10.1007/s12666-015-0763-x

9. “Electrophoretic deposition of Cu-SiO2 coatings by DC and pulsed DC for enhanced surface mechanical properties”, H.S. Maharana, S. Lakra, **S. Pal**, and A. Basu, **Journal of Materials Engineering and Performance**, Vol. 25, No. 1, pp. 327- 337(2016). DOI: https://doi.org/10.1007/s11665-015-1834-1

8. “Surface-Mechanical Properties of Electrodeposited Cu-Al2O3 Composite Coating and Effects of Processing Parameters”. HS Maharana, A Ashok, **S Pal**, A Basu, **Metallurgical and Materials Transactions A**, 47A, pp. 388—399 (2016). DOI:https://doi.org/10.1007/s11661-015-3238-0

7. ”Effect of basicity, Al2O3 and MgO content on the characteristic temperatures of the CaO-MgO-SiO2-Al2O3 high alumina quaternary slag system”. T. Trinath, N. Yedla, S. Sarkar, **S Pal**, **Metallurgical Research Technology**, Vol. 113(5), pp. 501 (2016).DOI: https://doi.org/10.1051/metal/2016015

6. ”Experimental and atomistic simulation based study of W based alloys synthesized by mechanical alloying” A. Patra, M. Meraj, S. Pal, N. Yedla and S.K. Karak, S. Pal, **International Journal of Refractory Metals and Hard Materials**, Vol. 58, pp. 57-67 (2016).DOI: https://doi.org/10.1016/j.ijrmhm.2016.04.002

2015:

5.”Asymmetry in steel welds with dissimilar amounts of sulfur”, H. L. Wei, **S. Pal**, V. Manvatkar, T. J. Lienert, and T. DebRoy. **Scripta Materialia**, Vol. 108, pp. 88- 91 (2015). DOI: https://doi.org/10.1016/j.scriptamat.2015.06.024

4. “The effect of nano-void on deformation behaviour of Al-Cu intermetallic thin film compounds”, N. Yedla, M. Meraj, P. Gupta, V. Sarat, A. J. Kabi and **S Pal (Corresponding Author)**, **Metallurgical Research Technology**, Vol. 112, pp. 505 (2015).
DOI: https://doi.org/10.1051/metal/2015033

2014:

3. ”Design of methane hydrate inhibitor molecule using Density Functional Theory.” **S Pal (Corresponding Author)** and T. K. Kundu, **Journal of Cluster Science**, Vol. 2, pp. 551-

563(2015).DOI:https://doi.org/10.1007/s10876-014-0826-x

2013:

2. "Pentagonal dodecahedron methane hydrate cage and methanol system - an Ab initio study" by **S Pal (Corresponding Author)**, T. K. Kundu, **Journal of Chemical Science**, Vol. 125, pp. 379–385 (2013).DOI: https://doi.org/10.1007/s12039-013-0392-z

1. "DFT based inhibitor and promoter selection criteria for pentagonal dodecahedron methane hydrate cage" **S Pal (Corresponding Author)**, T. K. Kundu, **Journal of Chemical Science**, Vol. 125, pp. 1259 -1266 (2013). DOI:https://doi.org/10.1007/s12039-013-0470-2

Conference Presentations

1. "An anomaly in creep property dependence on grain size for ultrafine grain nanocrystalline Nickel at higher creep temperature", Md. Meraj (Presenter), Snehanshu Pal, 2nd International Conference on Science and Engineering of Materials (ICSEM-2018), January 6-8, 2018, Sharda University (India).

2. "Effect of temperature on creep behavior of nanocrystalline Ni having multimodal grain distribution with pre- existing crack", Md. Meraj (Presenter), Snehanshu Pal, The 9th International Conference on Materials for Advanced Technologies (ICMAT-2017), June 18-23, 2017, Suntec Exhibition Center (Singapore).

3. "Analysis of deformation behaviour of Al-Ni-Co thin film during nanoindentation: A Molecular Dynamics study", K. Vijay Reddy (Presenter), Snehanshu Pal, 17th International Conference on Thin Films (ICTF-2017), November 13-17, 2017, CSIR-National Physical Laboratory, New Delhi (India).

4. "Molecular Dynamics simulation based study of the tensile loading behaviour of Silicene", B.S.K. Gargeya (Presenter), Snehanshu Pal, International Conference on Nanotechnology: Ideas, Innovations Initiatives (ICN:3I-2017), December 6-8, 2017, Indian Institute of Technology Roorkee (India).

5. "An atomistic simulation based investigation on the influence of Zr addition on deformation behavior of nanocrystalline Ni", Md. Meraj (Presenter), B.S.K. Gargeya, K. Vijay Reddy, Snehanshu Pal, 10th International Conference on Precision, Meso, Micro and Nano Engineering (COPEN 10), December 7-9, 2017, Indian Institute of Technology Madras (India).

6. "The Effect of Temperature on Creep Behaviour of Porous (1 at.Crystalline Nickel", M. Meraj (presenter) and S. Pal (Corresponding Author), 7th International Conference on Creep, Fatigue and Creep - Fatigue Interaction (CF-7)-2016, January 19-22, 2016, Indira Gandhi Centre for Atomic Research Kalpakkam (India).

7. "Deformation of Ni20W20Cu20Fe20Mo20 high entropy alloy for tensile followed by compressive and compressive followed by tensile loading: A molecular dynamics simulation based study", M. Meraj (presenter) and S. Pal (Corresponding Author) , 5th National Conference on Processing Characterization of materials 12-13th December, 2015 National Institute of Technology, Rourkela (India).

8. "Multiphase Computational Fluid Dynamics (CFD) modeling study of slopping behavior during basic oxygen steel making (BOS) process", S. Pal (presenter and Corresponding Author) , V. Kumari, R. Kumar and N. Yedla, KomPlasTech 2015- XXII International Conference Computer Methods in Materials Technology - January 11 -14, 2015, Krynica-Zdrój (Poland)

9. “Molecular Dynamics Studies on the Prediction of Interface Strength of Cu (metal)-CuZr (metallic glass) Metal Matrix Composites”, N. Yedla (presenter), R. Nalla, S. Pal, P. Gupta and M. Meraj, 8th International Conference on Materials for Advanced Technologies of the Materials Research Society of Singapore IUMRS – International Conference in Asia (ICMAT2015 IUMRS-ICA2015), 28 June - 3 July 2015, Suntec (Singapore).

10. ”Theoretical study of methanol as inhibitor and cyclopentane as stabilizer of dodecahedron methane hydrate cage.” S. Pal (presenter and Corresponding Author), and T. K. Kundu. In IOP Conference Series: Materials Science and Engineering, vol. 73, no. 1, p. 012081. IOP Publishing, 2015.

11. ”Density Functional Theory Study of Methane Encapsulation in Different Clathrate Hydrate Cage Structure” by S. Pal (presenter and Corresponding Author) ,and T. K. Kundu International Conference on Advances in Materials and Materials Processing (ICAMMP) 2011 Oral Presentation Volume (2011)

12. ”Comparative Stability Analysis of Different Methane Hydrates Structures Using Density Functional Theory” by S. Pal and T. K. Kundu, NMD ATM 2011

13. ”Fluid Flow Behavior of LD Converters Using Different” - e Turbulence Model” By T. K. Kundu , S. Pal (presenter and Corresponding Author) ,NMD ATM 2010 Page 77 (2010)

14. ”ANN Modeling For Prediction of Phosphorus, Carbon And Temperatures in LD Converter” by T. K. Kundu, S. Pal (presenter and Corresponding Author) ,NMD ATM 2010 Poster Volume, pp. 77 (2010)

Professional Membership

1. Life member in The Indian Institute of Metals (Membership No. LM55478)

2. Life member in Institution of Engineers (Membership No. AM1707232)

3. Associate Member - The Institute of Indian Foundrymen (Membership No. M/20549/E/HOW)

Workshop Attended

1st - 5th July 2014	Faculty Development Program in Pedagogy and E-learning Technology **National Institute Of Technology**, Rourkela,India
4th - 5th August 2015	National Workshop on Technology Enabled Learning (TECHEL - 2015) **Organized by A N Khosla Centre for Technology Learning, National Institute of Technology**, Rourkela,India

Team Player and leadership Skill

1. Organized National Conference of Processing Characterization Materials (NCPCM) 2014 conference seminar as a co-convener and treasurer in Metallurgical and Materials Engineering Department of National Institute of Technology Rourkela, India.
2. Organized Research Scholar Day 2011 conference seminar as a convener in Metallurgical and Materials Engineering Department of Indian Institute of Technology Kharagpur,

India.

Administrative Responsibilities

•Associate Dean (International Relation) ,Indian Institute of Engineering Science and Technology, Government of India, Shibpur, (Aril'2025 – Ongoing)

•Member of Institute Academic Program Oversight Committee - National Institute of Technology Rourkela (August'2016 – July'2019)

•Faculty Coordinator - Student Council Centre, National Institute of Technology Rourkela (July'2018 – June'2020)

•Faculty Advisor for B. Tech students of Metallurgical and Materials Engineering Department, National Institute of Technology Rourkela (July'2014 – June'2019)

•Worked as an Assistant Warden for a hostel having 1200 boarders in National Institute of Technology Rourkela (July'2015 – June'2017)

•Professor –in –Charge for Departmental Website of Metallurgical and Materials Engineering Department, National Institute of Technology Rourkela (July'2015 – June'2017)

•Member of disciplinary committee of Institute Hall Management Centre - National Institute of Technology Rourkela (August'2016 – June'2017)

•Member of purchase committee of Institute Hall Management Centre - National Institute of Technology Rourkela (August'2015 – June'2016)

Technical Software Skills

Programming Languages	FORTRAN, C, C++, Matlab,Python
Data Science:	Material Informatics , Machine Learning and Deep Learning
Artificial Intelligence Tools	ChatGpt, Gemini, Google NotebookLM, JAX (high-performance scientific ML),Vibe Coding with Google AI studio
Operating System:	Windows and Linux
Atomistic and Molecular Simulation Packages:	Gaussian 09, Lammps, Ovito
Computational Fluid Dynamics Package:	Ansys Fluent

Short Term courses/ Conferences Organized as Course coordinator or Convener

Date	Topic	Type
18-20 Dec 2020	Conference on Processing and Characterization of Materials (CPCM 2020)	Conference
14-18 June 2021	A Five Day Online AICTE Training and Learning (ATAL) Academic FDP Program On "Cultivating Excellence in Implementation of Computational Science for Scientific and Technological Innovations"	Workshop
22-26 Sep 2020	Molecular Modelling of Materials and Biological Macro Molecules	Workshop
01-05 Nov 2017	5 Day Workshop on Computational Techniques and Mathematical Modelling (CTMM-17) for Academia and Industry	Workshop

External Expert Evaluator Roles for Academic purpose (Invited/Nominated)

1. Act as **PhD Thesis External Examiner**, **Indian Institute of Technology Madras**, India, in the year of 2021 : Evaluated doctoral dissertation and provided independent assessment
2. Act as **PhD Thesis External Examiner**, **Indira Gandhi Centre for Atomic Research, Kalpakkam,** India, in the year of 2025 : Evaluated doctoral dissertation and provided independent assessment
3. Act as **M. Tech. Thesis External Examiner**, Metallurgical and Materials Engineering at **Indian Institute of Technology Kharagpur**, in the year of 2018 and 2024: Evaluated M. Tech. dissertation and provided independent assessment
4. Act as **External Expert in the Artificial Intelligence domain** of Peer Review Committee Meeting for the proposed project titled "Design and Development of Turret Gun system with Servo-Based Auto Target Tracking and Locking System (ATTALS) for 30mm 2A42 Cannon" held on 02nd March 2023 at **Armament Research and Development Establishment, Pune (Defence Research and Development Organisation (DRDO), Government of India)**

Declaration

I declare that all the information of my resume is correct as per my knowledge.

(Dr. Snehanshu Pal)