Curriculum vitae with track record

Personal information

First name, Surname:	**TARUN KUMAR KUNDU**		
Date of birth:	9th November, 1974	Sex:	MALE
Nationality:	INDIAN		
Researcher unique identifier(s) (ORCID.):	0000-0003-3853-4078		
URL for personal website:	http://www.iitkgp.ac.in/department/MT/faculty/mt-tkkundu		

Education

Year	Faculty/department - University/institution - Country
2004	**Ph.D**: Department of Metallurgical Engineering and Geosciences, Luleå University of Technology, Luleå, Sweden
1999	**ME** (Master of Engineering): Metallurgy, Indian Institute of Science, Bengaluru (Bangalore), India
1997	**BE** (Bachelor of Engineering), Metallurgical Engineering, Regional Engineering College (currently National Institute of Technology) Durgapur, West Bengal, India.

Positions - current and previous

Year	Job title – Employer - Country
2018 - present	Professor, Department of Metallurgical and Materials Engineering, Indian Institute of Technology Kharagpur, INDIA
2014–2018	Associate Professor, Department of Metallurgical and Materials Engineering, Indian Institute of Technology Kharagpur, INDIA
2006–2014	Assistant Professor, Department of Metallurgical and Materials Engineering, Indian Institute of Technology Kharagpur, INDIA
2004–2006	Post-Doctoral Fellow, Department of Mathematics, Luleå University of Technology, Sweden

Project management experience

Year	Project owner - Project - Role - Funder
2016-2021	IIT Kharagpur - Development of pilot scale palletisation technology for Indian geothitic/hematite ore with varying degree of fineness - Co-Principal Investigator - Ministry of Steel, Government of India
2015-2022	IIT Kharagpur- Hybrid Sodium ion Cell/Super Capacitor Packs for Light Electric Vehicles - Co-Principal Investigator - MHRD, Government of India
2012-2015	IIT Kharagpur - Development of pilot scale palletisation technology for Indian geothitic/hematite ore with varying degree of fineness - Principal Investigator - MINISTRY OF STEEL, Government of India
2010-2013	IIT Kharagpur - Atomistic Simulations of Gas Hydrates and Stabilizer/Inhibitor Design - Principal Investigator - Ministry of Earth Sciences, Government of India
2007-2010	IIT Kharagpur - Solvent Extraction Studies for High Value Metals by Ionic Liquids in Mixer-Settler Unit: Experimentation and Molecular Modeling - Principal Investigator - ISIRD, Indian Institute of Technology Kharagpur

Supervision of students

Master's	Ph.D	University/institution - Country
22 (2 ongoing)	**16** (11 ongoing, 3 completed, 2 submitted)	Indian Institute of Technology Kharagpur, INDIA

Other relevant professional experiences

Year	Description - Role
2018-	Co-ordinator, Post Graduate Studies, Department of Metallurgical and Materials Engineering, Indian Institute of Technology Kharagpur.
2007 -	In-Charge of Thermodynamic and Materials Processing Laboratory, Department of Metallurgical and Materials Engineering, Indian Institute of Technology Kharagpur.
2010-2018	Course convenor and Faculty Adviser for Master of Technology Program, Department of Metallurgical and Materials Engineering, Indian Institute of Technology Kharagpur
2014-2017	Assistant Warden, J.C Bose Hall of Residence, Indian Institute of Technology Kharagpur
2007-2021	Life Member and Paper Setter, Indian Institute of Metal, India
2007-2018	Member in Technical Committee: Congress Of Metallurgical Professionals invOlving Students, Industry & Teachers (COMPOSIT)
2011 & 2016	Member in Technical Committee: International Conference on Advances in Materials and Materials Processing (ICAMMP)
2014-2018	Member in Technical Committee: National Conference on Processing and Characterization of Materials (NCPCM)
2016 & 2019	Review board member for two Ph.D theses examination, CSIR-National Chemical Laboratory, Pune, India
2021	Review board member for Ph.D thesis examination, Indian Institute of Technology Bhubanewar, India
2007 -2021	**COURSES TEACHING/TAUGHT** 1. PRINCIPLES OF EXTRACTIVE METALLURGY 2. METALLURGICAL THERMODYNAMICS AND KINETICS Laboratory 3. TRANSPORT PHENOMENA IN METALLURGICAL PROCESSES 4. COMPUTER APPLICATIONS IN METALLURGICAL PROCESSES 5. ATOMISTIC MODELLING OF MATERIALS 6. PRINCIPLES OF IRON MAKING 7. EXTRACTIVE METALLURGY OF NON-FERROUS METALS

Track record

The total *number* of publications: **67 (Journal Papers: 46, Book Chapters: 5, Conference Proceedings: 16), 5 papers under review**

- **<u>Publications in Referred International Journals</u>**

1. Density functional theory-based analyses on selective gas separation by β-PVDF-supported ionic liquid membranes, Ranjini Sarkar and **T. K. Kundu**, Journal of Molecular Graphics and Modelling, 108, 108004, (2021).
2. Investigation of lanthanide complexation with acetohydroxamic acid in nitrate medium: experimental and DFT studies, A Pati, A Bhattacharyya, P. K Pujari, S. Pal, **T. K. Kundu**, Journal of Chemical Sciences 133 (3), 1-15, (2021).
3. Lanthanum ions decorated 2-dimensional g-C_3N_4 for ciprofloxacin photodegradation, S. K. Kuila, D.K Gorai, B. Gupta, A. K. Gupta, C. S. Tiwary, **T. K. Kundu**, Chemosphere 268, 128780, (2021).
4. First principle study of lithium and phosphorus co-doped graphitic carbon nitride as a nonlinear optical material, D. K. Gorai, **T. K. Kundu**, Materials Today Communications 26, 101911, (2021).
5. The role of density reduction in lithiated amorphous silicon: Molecular dynamics and ab-initio studies, J. K. Dora, C. Saraswat, A. Gour, S. Ghosh, N. Yedla, **T. K. Kundu**, Materials Today: Proceedings 44, 3075-3078, (2021).
6. Photocatalytic dye degradation under sunlight irradiation using cerium ion adsorbed two-dimensional graphitic carbon nitride, S. K. Kuila, R. Sarkar, P. Kumbhakar, P. Kumbhakar, C. S. Tiwary, **T. K. Kundu**, Journal of Environmental Chemical Engineering 8 (4), 103942, (2020).
7. Hydrogen bond interactions of hydrated aluminum nitrate with PVDF , PVDF-TrFE, and PVDF-HFP : A density functional theory-based illustration, Ranjini Sarkar, **T. K. Kundu**, International Journal of Quantum Chemistry 120 (17), 1-23, (2020).

8. Density functional theory based studies on the adsorption of rare-earth ions from hydrated nitrate salt solutions on g-C_3N_4 monolayer surface, R. Sarkar, S. Kumari, **T. K. Kundu**, Journal of Molecular Graphics and Modelling 97, 107577, (2020).
9. Influence of Pt and P doping on the performance of g-C_3N_4 monolayer, D. K. Gorai, **T. K. Kundu**, Materials and Manufacturing Processes 35 (6), 625-634, (2020).
10. A facile and green synthesis approach to derive highly stable SiO x-hard carbon based nanocomposites for use as the anode in lithium-ion batteries, J. K. Dora, D. Nayak, S. Ghosh, V. Adyam, N. Yedla, **T. K. Kundu**, Sustainable Energy & Fuels 4 (12), 6054-6065, (2020).
11. First Principle Study of Na and P Co-Doped Heptazine Based Monolayer g-C_3N_4, D. K. Gorai, **T. K. Kundu**, Materials Science Forum 978, 369-376, (2020).
12. Quantum chemical calculation based investigation of synergistic chelating between multiple hydroxyamide ligands and La^{3+} ion, A. Pati, **T. K. Kundu**, S Pal, Computational and Theoretical Chemistry 1170, 112643, (2019).
13. Nonbonding interaction analyses on PVDF/[BMIM][BF_4] complex system in gas and solution phase, R. Sarkar, **T. K Kundu**, Journal of molecular modeling 25 (5), 1-27, (2019).
14. Density functional theory studies on PVDF/ionic liquid composite systems, Ranjini Sarkar and **T. K. Kundu,** *Journal of Chemical Sciences* 130 (115), 10.1007/s12039-018-1522-4. (2018).
15. Adsorption Studies of Gadolinium ion on Graphitic Carbon Nitride, S. K. Kuila and **T. K. Kundu**, IOP Conference Series: Materials Science and Engineering 338 (1), 012006, (2018).
16. Density Functional Theory Study of Structural and Electronic Properties of γ'-Ni_3Al and γ''-Ni_3Nb, D. K. Gorai and **T. K. Kundu**, IOP Conference Series: Materials Science and Engineering 338 (1), 012041, (2018).
17. DFT Studies on Interaction between Lanthanum and Hydroxyamide, A. Pati, **T. K. Kundu** and S. Pal, IOP Conference Series: Materials Science and Engineering 338 (1), 012025, (2018).
18. A DFT+ U study of the catalytic activity of lanthanum nickelate, D. Misra and **T. K. Kundu,** *TheEuropean Physical Journal* B 90 (7), 135, (2017).
19. Strain-Controlled Transport Mechanism in Strongly Correlated $LaNiO_3$, D Misra, and **T. K. Kundu,** *Journal of Electronic Materials* 46 (1), 150-157, (2017).
20. Transport properties and metal–insulator transition in oxygen deficient $LaNiO_3$: a density functional theory study, D. Misra, and **T. K. Kundu,** *Materials Research Express* 3 (9), 095701, (2016).
21. Effect of strain on the optical properties of $LaNiO_3$: A first-principle study, D. Misra and **T. K. Kundu,** *Computational Materials Science* 112, 113-119, (2016).
22. Oxygen vacancy induced metal-insulator transition in $LaNiO_3$, D. Misra and **T. K. Kundu,** *The European Physical Journal B*, 89:4, https://doi.org/10.1140/epjb/e2015-60714-0 (2016).
23. A first-principle study of the optical properties of pure and doped $LaNiO_3$, D. Misra and **T. K. Kundu,** Advanced Materials Letters 7 (5), 344-348, (2016).
24. Cellular Automata Modeling of Decarburization of Metal Droplets in Basic Oxygen Steelmaking, Ankit and **T. K. Kundu**, IOP Conference Series: Materials Science and Engineering 115, 012001, (2016).
25. Design of Methane Hydrate Inhibitor Molecule Using Density Functional Theory, S. Pal and **T. K. Kundu,** *Journal of Cluster Science,* Vol 26, Issue 2, pp 551–563, (2015).
26. Development of High Capacity $Na_{0.7}(Ni_{0.4}Mn_{0.4}Co_{0.1}Fe_{0.1})O_2$ Cathode Material for Sodium Ion Batteries, **T. K. Kundu** and Chandra Kant Kaithwas, IOP Conference Series: Materials Science and Engineering 75 (1), 012008, (2015).
27. Modeling of Dephosphorization using Bloated Droplet Theory in Basic Oxygen Steelmaking, **T. K. Kundu** and Ankit, IOP Conference Series: Materials Science and Engineering 75 (1), 012022, (2015).
28. Theoretical study of methanol as inhibitor and cyclopentane as stabilizer of dodecahedron methane hydrate cage, S Pal and **T. K. Kundu**, IOP Conference Series: Materials Science and Engineering 73 (1), 012081, (2015).
29. The Effect of Methanol on 512 Methane Hydrate Cage Cluster – A Molecular Dynamics Study, S. Pal and **T. K. Kundu**, *Journal of Petroleum Engineering and Technology*, vol 4, issue 2, pp 16-24, (2014).
30. Natural Bond Orbital, Bond Order and Frequency based Study of Hydrogen Bond Formation in Different Glycols-Water Complex, S. Pal and **T. K. Kundu,** *Journal of Modern Chemistry & Chemical Technology* 4 (1), 1-20 (2013).

31. Stability analysis and frontier orbital study of different glycol and water complex, S. Pal and **T. K. Kundu,** *ISRN Physical Chemistry*, Article ID 753139, http://dx.doi.org/10.1155/2013/753139, (2013).
32. Pentagonal dodecahedron methane hydrate cage and methanol system—An ab initio study, S Pal and **T. K. Kundu,** *Journal of Chemical Sciences,* 125 (2), 379 (2013).
33. DFT-based inhibitor and promoter selection criteria for pentagonal dodecahedron methane hydrate cage, Snehanshu Pal and **T. K. Kundu,** *Journal of Chemical Sciences,* vol. 125, No. 5, pp. 1259–1266 (2013).
34. Drain Rate and Liquid Level Simulation in Blast Furnace Hearth Using Plant Data, H. Upadhyay and **T. K. Kundu,** *ISRN Metallurgy*, Article ID 960210, http://dx.doi.org/10.1155/2013/960210 (2013).
35. Stability analysis and Frontier Orbital Study of Different Glycol and Water Complex, Snehanshu Pal and **T. K. Kundu,** *ISRN Physical Chemistry*, ID 753139, p 1-16 (2013).
36. Theoretical study of hydrogen bond formation in chitosan and pentagonal dodecahedron methane hydrate cage structure, Snehanshu Pal and **T. K. Kundu** *Chemical Science Transaction*, vol. 2, no. 2, p 447-454 (2013).
37. Pentagonal dodecahedron methane hydrate cage and methanol system - an Ab initio study, Snehanshu Pal and **T. K. Kundu,** *Journal of Chemical Sciences*, v**.** 125, N. 2, p 379 (2013).
38. Natural Bond Orbital Analysis, Bond order and Frequency Calculation based Study of Hydrogen Bond Formation in Different Glycols and Water Complex, Snehanshu Pal and **T. K. Kundu,** *Journal of Modern Chemistry and Chemical Technology*, vol. 4, no. 1, p1-20 (2013).
39. Dodecahedron Methane Hydrate Cage Structure – An Ab initio Study, Snehanshu Pal and **T. K. Kundu,** *Journal of Petroleum Engineering and Technology*, vol. 2, no. 1, p 22-35 (2012).
40. Theoretical Prediction of Maximum Number of Methane Molecule Accommodation in Unit Cages of S-I Clathrate Structure, Snehanshu Pal and T**. K. Kundu,** *Journal of Petroleum Engineering and Technology*, vol. 2, no. 2, p 40-46 (2012).
41. Methane encapsulation in $5^{12}6^4$ clathrate cage - a theoretical study, Snehanshu Pal and **T. K. Kundu,** *Journal of Petroleum Engineering and Technology*, vol. 2, no. 3, p 1-8 (2012).
42. Theoretical study of hydrogen bond formation in trimethylene glycol-water complex, Snehanshu Pal and **T. K. Kundu,** *ISRN Physical chemistry*, ID 570394, p 1-12 (2012).
43. Atomistic simulation studies of magnetite surface structures and adsorption behavior in the presence of molecular and dissociated water and formic acid, **T. K Kundu**, K. H.Rao, and S. C Parker, *Journal of Colloid and Interface Science*, v 295, No 2, p 364-3 (2006).
44. Competitive adsorption on wollastonite: an atomistic simulation approach, **T. K Kundu**, K. H. Rao, and S. C Parker, *Journal of Physical Chemistry Part B: Condensed Matter, Materials, Surfaces, Interfaces & Biophysica*, v. 109 (22), p 11286 (2005).
45. Atomistic simulation of the surface structure of wollastonite, **T. K Kundu**, K. H. Rao, and S.C. Parker, *Chemical Physics Letters*, v. 377, N.1-2, p 81 (2003).
46. Atomistic simulation of the surface structure of wollastonite and adsorption phenomena relevant to flotation, **T. K. Kundu,** K. Hanumantha Rao, S. C. Parker, *International Journal of Mineral Processing*, v.72, I. 1-4, p. 111 (2003).

Publication in Book Chapters

1. Effect of Strain on the Physical Properties of Lanthanum Nickelate, D. Misra, **T. K. Kundu** and Ankit, TMS (The Minerals, Metals & Materials Society), 145 Annual Meeting Supplemental Proceedings 2016, pp 247-252, Springer International Publishing AG.
2. CFD Analysis to Estimate Refractory Erosion/scab Formation on Blast Furnace Hearth Wall, Hamant Upadhyay and **T. K. Kundu,** p-22-28, Jindal Tech, Issue 2, 2013.
3. Hot Metal Temperature Variation during Blast Furnace Tapping, Hamant Upadhyay and **T. K. Kundu,** p-67-72, Jindal Tech, Issue 2, 2013.
4. Molecular Modeling of Mineral Surface Reactions in Flotation, K Hanumantha Rao, **T. K. Kundu** and S. C. Parker, *Book Title: Molecular Modeling for the Design of Novel Performance Chemicals and Materials,* Pages 65-105, Taylor and Francis (CRC Press), **2012**.
5. CFD Modeling of Fluid Flow Behavior and Bath Surface Deformation in LD Converter, **T. K. Kundu**, S. Pal, *Book Title: CFD Modeling and Simulation in Materials Processing*, Pages 319-326, John Wiley & Sons Inc., **2012.**

Publications in International Conference Proceedings

1. Effect of ionic liquid addition on PVDF - a density functional theory study, T. K. Kundu, Ranjini Sarkar KomPlasTech, 13– 16 Jan, Zakopane, Poland (2019).

2. Dispersion Corrected Density Functional Theory Studies on PVDF/Hydrated Aluminium Nitrate Composite System, Ranjini Sarkar and **T. K. Kundu**, TMS Annual Meeting & Exhibition, Symposium: Computational Design and Simulation of Materials, Phoenix, USA (2018).
3. Rare earth ions adsorption on ultrathin graphitic carbon nitride, S. K. Kuila, **T. K. Kundu**, Proceedings of the international meeting on energy storage devices and and industry-academia conclave, Roorkee (India) 2018.
4. Development and Application of Mathematical Models to Simulate Liquid Phase Accumulation, Drainage, and Heat Transfer in Blast Furnace Hearth, H. Upadhyay, D. Chandra, T. K. Kundu, *Sustainable Industrial Processing Summit. Vol. 1. Afonso Intl. Symp./Iron and Steel Making* (pp. 151-164). Montreal, Canada (2018).
5. A Density Functional Theory based Study of Lanthanum Nickelate, **T. K. Kundu** and D. Misra, International Conference on Recent Advances in Materials & Manufacturing Technologies (IMMT) BITS Pilani Dubai Campus, Dubai, United Arab Emirates. Dubai, UAE, (2017).
6. Density Functional Theory Studies on Derivative Mercaptobenzothiozole as Chelating Agent in Flotation, **T. K. Kundu,** *XIII International Seminar on Mineral Processing Technology,* Bhubaneshwar*,* **p-62,** (2013).
7. Density Functional Theory Study of Methane Encapsulation in Different Clathrate Hydrate Cage Structure, Snehanshu Pal and **T. K. Kundu,** *International Conference on Advances in Materials and Materials Processing (ICAMMP),* IIT Kharagpur, (2011).
8. Comparative stability analysis of different methane hydrate structures using Density Functional Theory, Snehanshu Pal and **T. K. Kundu,** *NMD ATM,* Hyderabad*,* p 65, (2011).
9. Fluid flow behavior of LD converters using different k - ε turbulence model, **T. K. Kundu** and Snehanshu Pal *NMD ATM,* Bangalore, p 77, (2010).
10. ANN modeling for prediction of phosphorus, carbon and temperatures in LD converter, **T. K. Kundu,** Snehanshu Pal, *NMD ATM,* Bangalore*,* poster p 77, (2010).
11. CFD modeling of bath surface deformation using volume of fluid method, **T. K. Kundu**, Snehanshu Pal, *NMD ATM,* Bangalore*,* poster p 78, (2010).
12. Atomistic simulation on the adsorption of water, methanoic acid and methylamine on pure and hydroxylated quartz, K. Hanumantha Rao, T. K. Kundu, Eric Forssberg *Proceedings of the XXIII International Mineral Processing Congress: Istanbul, Turkey*, p. 1729-1735, (2006).
13. Molecular modelling of mineral surface structures and adsorption phenomena in flotation, Rao, K. H, **Kundu, T. K**., Parker, S. C. and Forssberg, E. *Centenary of Flotation Symposium Proceedings.*, ID: 505086, p. 557 (2005).
14. Atomistic simulation studies of surface structure of hematite and magnetite crystals and adsorption behaviour of water *by* **Kundu, T. K**, Rao, K. H. and Parker, S.C., *International Seminar on Mineral Processing Technology*, p. 190-197 (2003).
15. Atomistic simulation techniques for designing mineral specific collector molecules in froth flotation, **Kundu, T. K**, Rao, K. H., Parker, S.C. and Forssberg, E., *International Seminar on Mineral Processing Technology*, Vol. 1, p. 272-287 (2002).
16. Atomistic simulation techniques for modelling mineral surface reactions, **Kundu, T. K**., Rao, K. H. And Parker, S. C., *Proceedings: Advances in the understanding of adsorption phenomena at solid/aqueous solution interfa*, p. 67-72 (2001).

- **Invited presentations:**

1. Presented Seminar (2hr) on 'Application of Density Function Theory toward Innovation in Material Science/Technology' as expert speaker under "Cultivating Excellence in Implementation of Computational Science for Scientific and Technological Innovations" approved for funding by AICTE Training And Learning (ATAL) Academy, Government of India, organised by NIT Rourkela, India (13-16 June, 2021).
2. Presented Seminar (2hr) on «Introduction to Density Function Theory and Its Application» as expert speaker under, TEQIP-III Webinar Workshop on "Molecular Modeling of Materials and Biological Macromolecules", 22-26 September-2020, NIT Rourkela.
3. Invited Speaker on «Computational Approach to material design» underClean Energy Materials Innovation Challenge IC 6, 21st -22nd February 2019 IIT Delhi, New Delhi, organised by Department of Science and Technology, Govornment of India.
4. Invited Speaker on Materials Informatics: General Introduction, TwinAIML Seminar, Centre of Excellence in Artificial Intelligence, Indian Institute of Technology Kharagpur, 17th March, 2021

- ***Fellowships, awards and prizes:***

Awarded "Vattenfalls Stipendium", 2002, for best Licentiate Thesis (published halfway to the completion of PhD).