Brief CV: Tarun Kumar Kundu

Name in Full and Designation: **Dr. Tarun Kumar Kundu, Associate Professor**

Address	Date of Birth:	9th NOVEMBER, 1974
Department of Metallurgical and Materials Engineering **Indian Institute of Technology Kharagpur, WB- 721302** **Tel: +91 3222 283296, Mob: 9434156371** **E-mail: tkkundu@metal.iitkgp.ernet.in**	**Nationality:**	**INDIAN**
	Category:	**GEN**

Educational Qualification:

B.E(Bachelor of Engineering)**, 1997, Metallurgical Engineering, Regional Engineering College** (currently **National Institute of Technology**) **Durgapur,** FIRST CLASS HONOURS, **78.9 %** marks (position 3rd).

M.E (Master of Engineering), **1999, Metallurgy, Indian Institute of Science, Bangalore**, FIRST CLASS, CGPA-**6.7/8.0** (position 3rd).

Ph.D (Doctor of Philosophy), **2004**, Thesis Title: ***Atomistic simulation techniques for modelling inorganic/organic interface and flotation collector design***, Agricola Research Centre, Department of Metallurgical Engineering and Geosciences, Luleå University of Technology, LULEÅ, Sweden.

Professional Experience:

Postdoctoral positions, October 2004 – December 2006, Dept. of Mathematics, Luleå University of Technology, LULEÅ, Sweden, under Prof. Sven Öberg, worked in areas of application of Density Functional Theory (DFT) for interfacial properties of magnetite nanoparticles and reagent design,

Assistant Professor, December 2006 – November 2014, Dept. of Metallurgical and Materials Engineering, Indian Institute of Technology Kharagpur.

Associate Professor, November 2014- continuing, Dept. of Metallurgical and Materials Engineering, Indian Institute of Technology Kharagpur

Specialization and Expertise: Energy materials, Modeling and Simulation of Materials and Processes, Synthesis of Materials and Characterization

Awards and Distinctions: Awarded "Vattenfalls Stipendium of 25000 Swedish Kronar", 2002 for best Licentiate Thesis (published halfway to the completion of PhD).

Publication in refereed journals: **25** published, **2** accepted
Publications in proceedings of seminars/conferences: **6**
Publications as book chapters: **2**
Guidance at doctoral level: **2** completed, **8** under progress
Guidance at masters level: **13** completed, **1** under progress

Major sponsored R&D projects completed/handled:

1. Development of pilot scale palletisation technology for Indian geothitic/hematite ore with varying degree of fineness (DDO), MINISTRY OF STEEL,Government of India, duration 42 months (01-04-2012 to 30-09-2015), amount: 89.42 lakhs (PI)

2. Atomistic Simulations of Gas Hydrates and Stabilizer/Inhibitor Design, Ministry of Earth Sciences, Government of India, duration 40 months (25-08-2010 31-12-2013) amount: 31.92 lakhs (PI)

3. Solvent Extraction Studies for High Value Metals by Ionic Liquids in Mixer-Settler Unit: Experimentation and Molecular Modeling ISIRD, Indian Institute of Technology Kharagpur, duration 36 months (07-12-2007 06-12-2010), amount: 4.15 lakhs

Peer-reviewed articles

01. 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).
02. 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).
03. 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).
04. 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).
05. Design of Methane Hydrate Inhibitor Molecule Using Density Functional Theory**,** S. Pal, **T. K. Kundu**, *Journal of Cluster Science*, ***2015***, 26(2), 551-563.
06. 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).
07. 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).
08. 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).
09. 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).
10. 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).
11. 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).
12. A First-principle Study of The Optical Properties of Pure and Doped $LaNiO_3$, **Tarun Kumar Kundu,** Debolina Misra, *Advanced Materials Letters*, 2016, **7**(5).

13. Oxygen vacancy induced metal-insulator transition in $LaNiO_3$, Debolina Misra, **Tarun Kumar Kundu**, *The European Physical Journal B*, ***2016***, ,
14. Effect of strain on the optical properties of $LaNiO_3$: A first-principle study, D. Misra**, T. K. Kundu**, *Computational Materials Science*, ***2016***, 112, part A, p113–119.
15. Drain Rate and Liquid Level Simulation in Blast Furnace Hearth Using Plant Data, Hemant Upadhyay and **T. K. Kundu,** *ISRN Metallurgy*, Vol. 2013, Article ID 960210, http://dx.doi.org/10.1155/2013/960210 (2013).
16. Theoretical study of methanol as inhibitor and cyclopentane as stabilizer of dodecahedron methane hydrate cage**,** Snehanshu Pal, **T. K. Kundu**, *IOP Conf. Series: Materials Science and Engineering*, ***2015***, 73, 012081.
17. The Effect of Methanol on 512 Methane Hydrate Cage Cluster–A Molecular Dynamics Study, S Pal, **T. K. Kundu**, *Journal of Petroleum Engineering & Technology*, **2014**, 4(2), p16.
18. 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).
19. 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).
20. 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).
21. 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**,** Chandra Kant Kaithwas, **T. K. Kundu**, *IOP Conf. Series: Materials Science and Engineering*, ***2015***, 75, 012008.
22. Cellular Automata Modeling of Decarburization of Metal Droplets in Basic Oxygen Steelmaking, Ankit, **T. K. Kundu,** *IOP Conf. Series: Materials Science and Engineering* (2016), **115,** 012001
23. Modeling of Dephosphorization using Bloated Droplet Theory in Basic Oxygen Steelmaking, Ankit, **T. K. Kundu**, *IOP Conf. Series: Materials Science and Engineering*, ***2015***, 75, 012022.

Accepted Articles:

01. **D.Misra and T. K. Kundu,** DFT+U based studies of strain-controlled transport properties in strongly correlated $LaNiO_3$, Journal of Electronic Materials, DOI: 10.1007/s11664-016-4889-3.

02. **D.Misra and T. K. Kundu,** Transport properties and metal-insulator transition in oxygen deficient $LaNiO_3$ a density functional theory study, Materials Research Express, IOP Publishing.

Book Chapters:

01. 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**.
02. 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.**