BIBEK DASH

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EMPLOYMENT HISTORY

Senior Scientist	CSIR-Institute of Minerals and Materials Technology, Bhubaneswar, Odisha	December 2019 - present
Scientist	CSIR-Institute of Minerals and Materials Technology, Bhubaneswar, Odisha	November 2015 - December 2019
Research Scholar	Indian Institute of Science (IISc), Bangalore, Karnataka	July 2014- November 2015
Process Engineer	Hindalco Industries Pvt. Ltd., Aditya Birla Group, Odisha	July 2010- June 2011

PROFESSIONAL SUMMARY

Bibek Dash is a Senior Scientist in the Process engineering & Instrumentation Department, CSIR IMMT. He obtained Bachelor of Technology (B.Tech) degree in Chemical Engineering (2010) from NIT Rourkela and Masters of Technology (M.Tech) degree in Chemical Engineering (2013) from IIT Delhi. He is pursuing his Doctor of Philosophy (PhD) degree in the Department of Chemical Engineering at IIT Bombay. He is recipient of the Young Researchers award in 2013 for best master's project work at IIT Delhi. His research focuses are to use first principle modeling such as Density Functional Theory (DFT) and Molecular Dynamics (MD) to understand and design advanced materials for sustainable energy, environmental applications and mineral processing technologies.

He has worked on projects funded by CSIR/SERB/Ministry of Steel/NMDC/Industry/etc. The current research activities include the design of novel high-performance adsorbent materials for toxic pollutants removal, organic porous materials for gas capture and storage, transition metal catalysts for carbon dioxide conversion to fuels and chemicals, development of efficient codes for calculating thermodynamic parameters relevant to experimental researchers, high capacity battery materials design and optimization using DFT and AI-based design, electrochemical carbon dioxide reduction to fuels and chemicals using novel metal-organic complexes, 2D materials hybrid structures and metal surfaces and flotation reagent design for efficient mineral flotation process.

Research Interests

- Novel high-performance adsorbent materials using low-cost/grade mineral ores for toxic heavy metals pollutants removal
- Computational design of organic porous nanomaterials for CO2 storage and capture and pollution reduction
- Design of transition metal based catalysts for catalytic process (electrochemical/photocatalytic)
- DFT and MD based advanced materials design for battery applications
- Novel flotation reagents design for low grade mineral ores/slimes/tailings using modeling
- Chemical Additives development for slurry transport and dewatering of iron ores and coal

EDUCATION

Doctor of Philosophy (Ph.D)	Department of Chemical Engineering, Indian Institute of Technology (IIT), Bombay, Maharashtra	continuing
Master of Technology (M.Tech)	Department of Chemical Engineering, Indian Institute of Technology (IIT), Delhi , Delhi	2013
Bachelors of Technology (B.Tech)	Department of Chemical Engineering, National Institute of Technology Rourkela, Odisha	2010

R&D PROJECTS

CURRENT PROJECTS

Sl. No.	**Title**	**Sponsoring Agency**	**Period**		**Amount (Rs in Lakhs)**
			From	**To**	
1.	Machine Learning based electrode material design for energy storage applications	CSIR-AI	2022	2024	79.05
2.	Development of Green Surfactants for Mineral Flotation and Flocculation: Molecular Level Design, Characterization, and Synthesis (GSMF)	CSIR-4M	2018	2024	80.00
3.	Fluorescent anti-corrosion coatings for early detection of failure via modeling and simulation	SERB	2024	2027	15.0

4.	Studies on feasibility of coal-water slurry preparation, transportation & dewatering of pulverized coal	CSIR-4M	2024	2026	
5.	Processes for high pure silica from the sad of waste overburden of lignite mines and value addition to magnesite-based low-grade mines resources	CSIR-FTT	2024	2026	200.0
6.	Simultaneous removal of CO2, SO2, and NOx from flue gas and their catalytic conversion into fuels and fertilizers	Ministry of Steel	2022	2024	
7.	Study the physical and mineralogical effect on the recovery of iron values from beneficiation plant residual fines/slimes/tailings and grade iron ore-an approach towards iron ore sustainability	Ministry of Steel	2024	2026	108.0

PROJECTS COMPLETED

Sl. No.	**Title**	**Sponsoring Agency**	**Period**		**Amount (Rs in Lakhs)**
			From	**To**	
1.	Molecular modeling studies on low cost mineral based adsorbents: Implication to fluoride and uranyl ion	CSIR	2018	2020	8.00
2.	Multiscale modeling and computational design of high-performance materials for remediation of polluted water	CSIR	2020	2022	30.00
3.	Modeling and optimization of screen performance for higher productivity at minimal misplacements	Tata Steel Ltd., Jamshedpur, Jharkhand	2018	2019	30.00
4.	Modeling and Optimization of High Concentration iron Ore fines/concentrate Slurry Pipelines for Indian Iron Ore Processing Industries	NMDC & Ministry of Steel, Govt. of India	2017	2020	425.00
5.	Challenges in recycling and material development from spent FCC catalyst	CSIR	2019	2021	10.00
6.	In-house development and fabrication of stirred mills for energy efficient processing of low grade ores	CSIR	2019	2021	60.00

7.	Multifunctional electrodes and electrolytes in future technologies	CSIR	2015	2017	15.00
8.	Synthesis of Smart Metal-Organic Porous Hybrid Materials as Renewable energy carrier modules	CSIR	2015	2017	15.00

PUBLICATIONS

Statistics on Publications

Total Citations generated	**192**
Total Impact factor generated	**44.5**
h-index	**7**
i10-index	**6**

JOURNALS

1. Kumar, N., Mishra, R. P., **Dash, B.**, Bastia, S., & Chaudhary, Y. S. (2023). The synergistic chemical coupling of nanostructured MoS2 with nitrogen-deficient 2-D triazine-based polymeric M-c3nx for efficient and selective CO2 photocatalytic conversion to CO. **Journal of Materials Chemistry A. (IF:11.9)**,11 (38), 20839-20853. https://doi.org/10.1039/d3ta03267a

2. Sohale, A. P., Janardanan, **Bibek Dash**, S., Yadav, D.., & Yadav, M. D. (2023). Dark fermentative Biohydrogen production: Recent advances and challenges. **Industrial & Engineering Chemistry Research (IF:4.2)**,62(37), 14755-14771. https://doi.org/10.1021/acs.iecr.3c01439

3. **Bibek Dash**, Sandeep K. Jena, Swagat S. Rath, Adsorption of Cr (III) and Cr (VI) ions on muscovite mica: Experimental and molecular modeling studies, **Journal of Molecular Liquids (IF:6.0)**, 357, 2022, 119116, https://doi.org/10.1016/j.molliq.2022.119116.

4. **Bibek Dash**, Swagat S. Rath, Density Functional Theory and Molecular Dynamics insights into the site-dependent adsorption of hydrogen fluoride on kaolinite, **Journal of Molecular Liquids (IF:6.0)**, 299, 2020, 112265, https://doi.org/10.1016/j.molliq.2019.112265

5. **Bibek Dash**, Barsha Dash, Swagat S. Rath, A thorough understanding of the adsorption of Ni (II), Cd (II) and Zn (II) on goethite using experiments and molecular dynamics simulation, **Separation and Purification Technology (IF:8.6)**, 240, 2020, 116649, https://doi.org/10.1016/j.seppur.2020.116649.

6. **Bibek Dash**, Carbon dioxide capture by nitrogen-containing organic materials – A density functional theory investigation, **Computational and Theoretical Chemistry (IF:2.8)** , 1128, 2018, 1-14, 2210-271X, https://doi.org/10.1016/j.comptc.2018.02.005.

7. **Bibek Dash**, Carbon dioxide capture using covalent organic frameworks (COFs) type material—a theoretical investigation. **Journal of Molecular Modeling (IF:2.2)** 24, 120 (2018). https://doi.org/10.1007/s00894-018-3646-3

8. **Bibek Dash** & Abhishek Kumar (2017) Nanofiltration for textile dye–water treatment: Experimental and parameter estimation studies using a spiral wound module and validation of the Spiegler–Kedem-based model, **Separation Science and Technology (IF:2.8)**, 52:7, 1216-1224, DOI: 10.1080/01496395.2017.1282965

BOOK CHAPTER

1. Shailesh K. Singh, Gourav Shrivastav, Tuhin S. Khan, **Bibek Dash**, Vivek K. Singh, Application of Molecular Dynamics and Calorimetry for Study and Characterization of Polymers, Editor(s): M.S.J. Hashmi, **Encyclopedia of Materials: Plastics and Polymers**, ***Elsevier,* 2022,** 555-564, ISBN 9780128232910, https://doi.org/10.1016/B978-0-12-820352-1.00278-9.

2. **Bibek Dash**, Barsha Dash, Manishkumar D Yadav, Bio-derived carbon nanostructures for environmental applications, **Bio-derived Carbon Nanostructures: Fundamentals, Synthesis and Applications**, ***Elsevier, 1st Edition 2024***, ISBN: 9780443135798

3. Nishtha Arora, Sachin Dua, S V Purohit, **Bibek Dash**, Manishkumar D. Yadav, Bikash Kumar Jena, T.Senthilkumar, Polymer Composites: Synthesis, Application, and Basic Theoretical Aspects, **Polymer Composites: From Computational to Experimental Aspects, *Springer Nature* 2024**, ISBN: 978-981-97-0887-1

CONFERENCE

1. Deepak Adhikari, Pradyut Sengupta, **Bibek Dash**, Mayadhar Debata, Ajit Panigrahi, Surojit Gupta, Engineered role of Cr and Cr2AlC on structure-property evolution of Cu alloys, Frontiers in Materials for Technological Applications FIMTA 2022, Bhubaneswar

2. G Hazare, S D Mohapatra, **Bibek Dash**, S S Rath, R K Dwari, Biomass residue and its synthesized derivatives as collector for the flotation of calcite-quartz system, Frontiers in Materials for Technological Applications FIMTA 2022, Bhubaneswar

3. Sudhanshu Ranjan, Anupam Biswas, Rahul Bhoi, Shradhanjali Sahoo, **Bibek Dash**, Curcumin, Eugenol and Nimbolide as potential ayurvedic anticancer drugs-A combined molecular docking

and DFT analysis, Frontiers in Materials for Technological Applications FIMTA 2022, Bhubaneswar

4. Ajay Verma, Amogh Raj, **Bibek Dash**, Manish Kumar Yadav, Evaluation of Thermodynamic Models for the Prediction of Solubility of Antibiotics In Various Solvents, IIChE CHEMCON 2021, Bhubaneswar

5. Ravi Gupta, **Bibek Dash**, Manish Kumar Yadav, Role of reducing agent concentration in tuning the number of layers of graphene oxide using improved Hummers method, IIChE CHEMCON 2021, Bhubaneswar

6. **Bibek Dash**, Barsha Dash, Swagat S. Rath, J. Das, Investigations of adsorption mechanisms of Ni, Cd and Zn on goethite mineral through Density functional theory and molecular dynamics simulations, Mineral Processing Technology MPT 2019, Hyderabad

7. **Bibek Dash**, Molecular Modeling studies of adsorption of toxic elements on low cost minerals, 3D-Experience Design Conference Dassault Systemes 2019, Bangalore

8. **Bibek Dash**, Removal of halide from water by spiral wound nanofiltration module, IIChE, CHEMCON 2012, Jalandhar

9. **Bibek Dash**, Dinesh Attarde, Investigation of suitable mass transport model of flat sheet membrane for osmotic power generation, IIChE, CHEMCON 2012, Jalandhar

SKILLS

Density functional theory (Planewave DFT, LCAO DFT), Molecular Dynamics simulations(MD), Monte Carlo simulations (Markov chain MC, Grand Canonical MC, Reverse Monte Carlo), Design of catalytic materials aided by mathematical modeling and experiments, computational catalysis for energy conversion applications, Structure-property relationships investigations for efficient adsorbent designs, CO2 to Fuels conversion

AWARDS & HONORS

- Recipient of the Young Researcher Award 2013 for best master's project work at IIT Delhi
- Best Poster award in competition at CHEMCON International Conference, 2021
- Joint Secretary and Executive Council Member (2015-2021), IIChE Bhubaneswar Regional Center