Supriti Dutta

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I am a Computational Researcher with expertise in catalysis. The goal of my research is to design novel, economical, and efficient electrocatalysts as well as photocatalysts for converting hazardous gases into value-added chemicals. I apply various tools of DFT and AIMD to design catalysts based on nanosheets, COFs, MOFs, alloy systems, heterointerfaces for industrially important catalytic reactions such as the hydrogen evolution reaction, oxygen reduction reaction, oxygen evolution reaction, reduction of carbon dioxide, nitrogen reduction to form ammonia and urea. I studied data-driven machine learning for finding efficient catalyst towards various energy conversion processes. I am currently working on discovering pseudocapacitor for suitable energy storage and thermal catalysis for decomposition of the toxic nerve agent Sarin.

Academic Record

2024 – present

Postdoctoral Research Associate
Chemical & Biomolecular Engineering Dept., University of California, Los Angeles (UCLA)

2018 - 2023

Ph.D. in Computational Materials Science
Theoretical Sciences Unit, Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore, India
Thesis Title: "Computational Studies on the Photo-Electrocatalytic Activity & Selectivity in Renewal Energy Conversion Processes"

2016 – 2018

M. Sc in chemistry (specialized in physical chemistry)
Visva-Bharati University, Santiniketan, India
Master's project: "Additive-Free Cobalt-catalysed hydrogenation of Esters to Alcohols"

2013 – 2016

B. Sc in chemistry with allied subjects Mathematics and Physics
Visva-Bharati University, Santiniketan, India

Research Topic

In my research, I primarily dealt with heterogeneous catalysis for various reactions such as oxygen evolution reaction (OER), oxygen reduction reaction (ORR), hydrogen evolution reaction (HER), water splitting, multifunctional activities (HER/OER/ORR), CO_2 reduction, Nitrogen reduction to form ammonia (NRR) and urea formation. I explored various materials like graphene-based systems, covalent organic frameworks, metal-alloy systems, heterointerface, carbon nitride nanosheets etc in my doctoral studies. By using quantum chemical calculations, I explored the mechanism of the reactions both thermodynamically and kinetically. I considered various types of descriptors like adsorption free energy, energy barrier, overpotential, onset potential, charge transfer, exchange current density, ESSI, DOS, BAND, d-band center, ICOHP to understand the origin of catalytic activity. I studied the scaling relationship and breaking of the scaling relationship also in a few works. Thus, in brief, I tried to provide a computational understanding of the mechanism and guiding design principle of economic and novel catalysts for a number of reactions of relevance to tackle the energy crisis in my PhD thesis. In the last few years, I have been also involved in multiple projects with experimental collaboration for understanding the origin of catalytic activity towards HER in alkaline medium, water splitting, OER, ORR etc. Currently I am working on an NSF project where we are especially interested in identifying pseudocapacitive materials with higher energy density and operation at higher potentials (vs. Li^+/Li) than the currently known pseudocapacitive materials. Also, I am exploring thermal catalysis for toxic nerve agent sarin decomposition in collaboration with US military.

Key points

- Experienced researcher in both Homogeneous and Heterogeneous Catalysis field by applying thermodynamic as well as kinetic approach.
- Designed many economical and efficient novel catalysts that can be applied to convert hazardous gases into energy fuels and explained the catalytic activity. Data-driven machine learning was also explored for finding efficient heterogeneous catalysts for various energy conversion processes.
- Self-motivated, enthusiastic, project designing capability, multitasking, team leader, flexibility to work, presentation skills with versatile project management ability.

Selected Research Publications

1. S. Das, S. Bhattacharjee, S. Mondal, S. Dutta, S K. Pati and S. Bhattacharyya, Bimetallic Zero-Valent Alloy with Measured High-Valent Surface States to Reinforce the Bifunctional Activity in Rechargeable Zinc-Air Batteries, *ACS Sustainable Chem. Eng*. 2021, 9 (44), 14868−14880
2. S. Dutta, P. Banerjee and S K. Pati, Computational Insight into TM−Nx Embedded Graphene Bifunctional Electrocatalysts for Oxygen Evolution and Reduction Reactions, *ACS Phys. Chem Au*, 2022, 2 (4), 305–312

3. S. Dutta and S K. Pati, Anchoring boron on a covalent organic framework as an efficient single atom metal-free photo-electrocatalyst for nitrogen fixation: a first-principles analysis, *Phys. Chem. Chem. Phys*., 2022, 24 (18), 10765-10774 (HOT ARTICLE)
4. S. Dutta and S K. Pati, Tetrazine Based Covalent Organic Framework as a Promising Metal-Free Photo & Electro-Catalyst for HER, *Catalysis Letters*, 2022, 152 (12), 3548–3557
5. M. Maji, N. Dihingia, S. Dutta, S. Parvin, S K. Pati and S. Bhattacharyya, Charge transfer modulated heterointerfaces for hydrogen production at all pH values, *J. Mater. Chem. A*, 2022, 10 (46), 24927-24937
6. S. Dutta and S K. Pati, Novel design of single transition metal atoms anchored on C_6N_6 nanosheet for electrochemical and photochemical N_2 reduction to Ammonia, *Catalysis Today*, 2022 (DOI: 10.1016/j.cattod.2022.06.019)
7. P. Sreejyothi, P. Sarkar, S. Dutta, A. Das, S K. Pati and S K. Mandal, Regioselective ring-opening of epoxides towards Markovnikov alcohols: A metal-free catalytic approach using abnormal N-heterocyclic carbene, Chemical Communications, 2022, 58(68), 9540-9543
8. S. Dutta and S K. Pati, Urea Production on Metal-Free Dual Silicon Doped C_9N_4 Nanosheet Under Ambient Conditions by Electrocatalysis: A First Principles Study, *ChemPhysChem*, 2023, 24(1), e202200453 (DOI: 10.1002/cphc.202200453)
9. S. Parvin, N. Bothra, S. Dutta, M. Majhi, A. Kumar, M. Mura, D K. Chaudhary, P. Rajput, M. Kumar, S K. Pati, and S. Bhattacharyya Inverse 'Intra-Lattice' Charge Transfer in Nickel-Molybdenum Dual Electrocatalysts Regulated by Under-coordinating the Molybdenum Center, *Chemical Science*, 2023, 14(11), 3056-3069
10. S. Mondal, S. Dutta, S. Mal, S K. Pati and S. Bhattacharyya, Nickel-Indium Heterogeneous Alloys with Minimized Lattice Mismatch for Alkaline Water Reduction, *Angewandte Chemie, 2023, 62(18), e202301269*
11. S. Dutta and S K. Pati, Boosting Photo-assisted efficient Electrochemical CO_2 Reduction Reaction on Transition Metal Single-Atom Catalysts Supported on C_6N_6 nanosheet: A Computational Study, *Phys. Chem. Chem. Phys*, 2023, *25 (23), 15788-15797*
12. A. Mondal, S. Dutta, S K. Pati and S. Bhattacharyya, Phase Transition from Dion Jacobson Hybrid Layered Double Perovskites to 1D Perovskites for Ultraviolet to Visible Photodetection, *Chemical Science, 2023, 14 (36), 9770-9779*
13. M Maji, S Dutta, R Jena, A Dey, TK Maji, SK Pati, S Bhattacharyya, Hydrogen Evolution in Neutral Media by Differential Intermediate Binding at Charge-Modulated Sites of a Bimetallic Alloy Electrocatalyst, *Angewandte Chemie International Edition, e202403697*
14. A. Garg, A. Saha, S. Dutta, S K. Pati, M. Eswaramoorthy, CNR Rao, High Ammonia Yield Rate from Dilute Nitrate Solution Using Cu(100)-Rich Foil: A Step Closer to Large-Scale Production, *ACS Applied Materials & Interfaces, 2024, 16 (28), 36392-36400*
15. L Sahoo, S Dutta, A Devi, S K. Pati and A P, Ligand Chain Length of Pt6(SR)12 Nanoclusters Controls the Hydrogen Evolution Efficiency, (*Nano Letters,* in press)

Packages

VASP, ASE, Gaussian, Quantum Espresso, SIESTA, Lobster, Materials Studio

Visualization and Plotting Software

Vesta, Xcrysden, Gaussview, xmgrace, Gnuplot, matplotlib, Origin, Mercury, VMD, Vaspkit, wxDragon, Chemcraft

Awards and Achievements

- Best poster award in Current Trends in Theoretical Chemistry (CTTC), 2020. (Oral presentation + poster)
- All India Rank 36 in Graduate Aptitude Test Engineering (GATE) in Chemistry, 2018.
- Joint five years research fellowship and lifetime lectureship award (all India rank 28) by Council of Scientific and Industrial Research (CSIR), India, 2017.
- UGC-JRF with AIR-88 rank in CSIR UGC NET in Chemical Science held on Dec 2016.
- Selected as Swami Vivekananda Merit-cum-Means Scholar.
- Five years INSPIRE scholarship awarded by Department of Science and Technology, India, 2013. Awarded to only the top 1% student in the country pursuing a career in basic science.
- District Topper during the Higher Secondary Examination, 2013.

Presentations

- Designing Catalysts on Computers (DCC) IACS, India (December 2022) (poster)
- 'Chemistry of Materials' conference in Kerala, India, (October 2022) (poster)
- Theoretical Science Unit Day, JNCASR (May 2022) (oral presentation)
- Theoretical Chemistry Symposium, IISER-Kolkata, India (December 2021) (poster)
- Theoretical Science Unit Day, JNCASR (May 2021) (poster)
- "Tetrazine Based Covalent Organic Framework as a Promising Metal-Free Photo and Electro-Catalyst for HER", Current Trends in Theoretical Chemistry (CTTC), BARC, Mumbai, India (October 2020) (poster + oral presentation)
- JNCASR Annual In-House Symposium, Bangalore, India, 2020 (poster)
- International Winter School on "Frontiers in Materials Science" (December 2019) (poster)

Other Merits

journal reviewer

2018-ongoing
PCCP, JPC C, JPC L

Teaching Experience

2019-2020 & 2020-2021
TA for teaching DFT to the Masters & Int. Ph.D. students and also performed tutorial classes for gaussian, gauss view.

Positions of responsibility

Volunteer in Student buddy programme, JNCASR (2019)
Students Representative for a year in JNCASR (2019-20)
Subject matter expertise for teaching in Chemistry.