

Dr. Suman Kalyan Sahoo

Assistant Professor

Computational Materials Chemistry Laboratory

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Education

- PhD 2015 - Visva-Bharati University, Santiniketan, India.
- MSc 2006 – Pt. Ravisankar Shukla University, Raipur, India.

Professional Experiences

- 2022- Present: Assistant Professor, CNMS, Jain University, India.
- 2021-2022: Guest Faculty, HNMG Central University, Srinagar, India.
- 2021-2022: Post-Doctoral Researcher, NTU, Taiwan.
- 2019-2021: Visiting Researcher, KTH, Stockholm, Sweden.
- 2016-2019: Post-Doctoral Researcher, POSTECH, Pohang, South Korea.
- 2015-2016: Research associate, Visva-Bharati University, Santiniketan, India.

Scholarastic Achievements:

- Awarded Senior Research Fellowship sponsored by Council of Scientific and Industrial Research (CSIR), India, 2012.
- Awarded Junior Research Fellowship sponsored by Board of Research in Nuclear Sciences (BRNS), India, 2009.
- Qualified joint CSIR-UGC National Eligibility Test (NET)-Dec 2006, Chemical Sciences.
- All India 461th rank in Graduate Aptitude Test for Engineers (GATE)-2007, Chemistry.

Membership of Professional societies:

Life member, Society of Material Chemistry, Mumbai, India.

Research funding

Project funding of 2 lakhs from CNMS, Jain University (2022-2023).

Leader and Supervision Experience

Doctoral research (PhD student): 1 started in January 2023

M.Sc. Project student: 1 started in 2023

Lead role in the setting up a CNMS-High performance computing (HPC) Cluster for the computational research. It is a new division to the center. The linux cluster setup consists of 1 Master node and 2 Compute nodes. All the nodes are connected to GigE Switch. Total CPU cores is 120.

Teaching Experience

Teaching modules of Analytical chemistry and Quantum chemistry to MSc students. Taking Data handling class for the PhD course work. Design Computational Chemistry Special paper for the PhD students.

Highlights of Faculty achievement

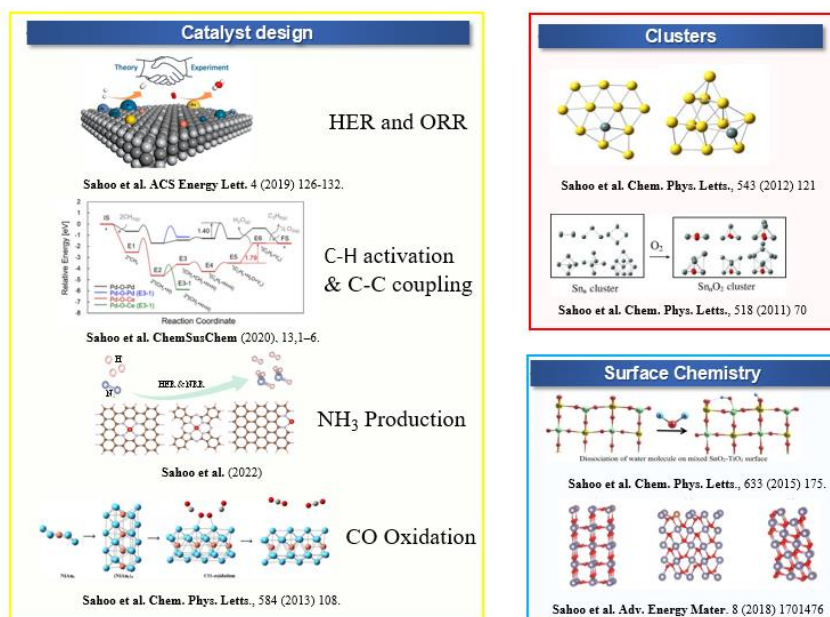
Sl No	Date of Completion of Ph.D.	Total no of Publications during Ph.D	Total no of publications Post Ph.D.	Total Teaching experience (years)	Total UG Teaching Experience (years)	Total PG Teaching Experience (years)	Total post Ph.D. Teaching Experience	Research Experience (years)
1	May. 2015	9	6	4	1	3	3	10

Research Activities: Dr. Suman Kalyan Sahoo

Welcome to **Computational Materials Chemistry Laboratory**

Performing computational and theoretical research (mainly density functional theory calculation) at CNMS with a broad range of interests in materials properties and studies on Heterogeneous Catalysts for Energy and Environmental Applications. Our main aim is to guide or complement experiment through high-throughput catalyst screening and elucidating the reaction mechanism. With the advance of computers and algorithms, before we start any experiment at laboratory to reach the desired product, we can feel this path with computer programs. Over the past few decades, among other theories Kohn–Sham density functional theory (DFT) is most widely used to find these reaction paths and develop catalyst materials for various applications on diverse reaction conditions. Understanding the nature at atomic level with DFT makes possible to provide fundamental information from the bottom-up approaches for designing new types of catalyst.

We use the state of the art electronic structure simulation tools and analysis to understand, design and discover materials for catalyzing chemical reactions such as CO oxidation reaction (auto-mobile exhaust catalyst), methane conversion, oxygen reduction and hydrogen evolution reactions (Fuel cell), nitrogen reduction reaction (ammonia synthesis), electrochemical synthesis of hydrogen peroxide and so on, for application in renewable energy technologies aiming green environment.



Publications:

1. Hemavathi N J, Chiranjib Majumder and Suman Kalyan Sahoo, Screening and investigation of ligand effect on TM single atom catalyst toward hydrogen evolution reaction: A DFT Study, submitted (2024).
2. Suman Kalyan Sahoo, Tore Brinck, Designing V single atom embedded carbon moiety for the electrocatalytic nitrogen reduction reaction by first principles study, submitted (2024).
3. Mukaddar Sk, Ibrarc, Saurabh Ghosh and Suman Kalyan Sahoo, A DFT study: Lead-free double perovskites halides (Rb/Cs)₂AgTlBr₆ for solar cell and green energy application, submitted (2024).
4. Revathi Kottapparaa, Hemavathi N J, Suman Kalyan Sahoo, Shajesh Palantavida and Baiju Kizhakkekilikoodayil Vijayan, Nickel sheathed copper nanowires with improved catalytic activity for the reduction of p-nitrophenol, submitted (2024).
5. Tore Brinck, Suman Kalyan Sahoo, Anomalous Pi-backbonding in Complexes between B (SiR₃)₃ and N₂: Catalytic Activation and the Breaking of Scaling Relations, Phys. Chem. Chem. Phys., 2023,25, 21006-21019.
6. Gihun Kwon, Dongjae Shin, Hojin Jeong, Suman Kalyan Sahoo, Jaeha Lee, Gunjoo Kim, Do Heui Kim, Jeong Woo Han and Hyunjoo Lee. Oxidative Methane Conversion to Ethane on Highly Oxidized Pd/CeO₂ Catalysts Below 400 °C. ChemSusChem 2020,13,1-6. (IF=7.96).
7. Suman Kalyan Sahoo, Youngjin Ye, Seonggyu Lee, Jinkyu Park, Hyunjoo Lee, Jinwoo Lee, and Jeong Woo Han. Rational Design of TiC-supported Single Atom Electrocatalysts for Hydrogen Evolution and Selective Oxygen Reduction Reactions. ACS Energy Lett. 4 (2019) 126-132. (IF=19.003).

8. Jiwhan Kim, Chi-Woo Roh, Suman Kalyan Sahoo, Sungeun Yang, Jeong Woo Han, and Hyunjoon Lee. Highly Durable Platinum Single Atom Alloy Catalyst for Electrochemical Reactions. *Adv. Energy Mater.* 8 (2018) 1701476. (I.F=25.24)
9. Santu Biswas, Anup Pramanik, Tasnim Ahmed, Suman Kalyan Sahoo, Pranab Sarkar. Superiority of D–A–D over D–A type of organic dyes for the application in dye-sensitized solar cell. *Chem. Phys. Letts.*, 649 (2016) 23. (I.F=2.02)
10. Suman Kalyan Sahoo, Sandeep Nigam, Pranab Sarkar & Chiranjib Majumder. Is mixed oxide of $\text{Sn}_x\text{Ti}_{1-x}\text{O}_2$ more effective for H_2O decomposition? A first Principles Study. *Chem. Phys. Letts.*, 633 (2015) 175. (I.F=2.02)
11. Sandeep Nigam, Suman Kalyan Sahoo, Pranab Sarkar & Chiranjib Majumder. Chair like NiAu_6 : Clusters assemblies and CO oxidation study by ab initio methods. *Chem. Phys. Letts.*, 584 (2013) 108. (I.F=2.02)
12. Suman Kalyan Sahoo, Sandeep Nigam, Pranab Sarkar & Chiranjib Majumder. Influence of Sn interaction on the structural evolution of Au clusters: A first principles study. *Chem. Phys. Letts.*, 543 (2012) 121. (I.F=2.02)
13. Suman Kalyan Sahoo, Sougata Pal, Pranab Sarkar & Chiranjib Majumder. Size dependent electronic structure of rutile TiO_2 quantum dots. *Chem. Phys. Letts.*, 516(2011)68. (I.F=2.02)
14. Suman Kalyan Sahoo, Sandeep Nigam, Pranab Sarkar & Chiranjib Majumder. Oxidation of tin clusters: A first principles study. *Chem. Phys. Letts.*, 518 (2011) 70. (I.F=2.02)
15. Suman Kalyan Sahoo, Sandeep Nigam, Pranab Sarkar, Chiranjib Majumder, “Transition metal dimer on Au (111) surface: A first principle study”, *AIP Conf. Proc.* 1447, 473 (2012).
16. Suman Kalyan Sahoo, Sandeep Nigam, Pranab Sarkar, Chiranjib Majumder, “DFT study of H_2O adsorption on TiO_2 (110) and SnO_2 (110) surfaces”, *AIP Conf. Proc.* 1512, 292 (2013).
17. Sandeep Nigam, Suman Kalyan Sahoo, Pranab Sarkar, Chiranjib Majumder, “Adsorption of Eu atom at the TiO_2 anatase (101) and rutile (110) surfaces”, *AIP Conf. Proc.* 1512, 290 (2013).
18. Sandeep Nigam, Suman Kalyan Sahoo, Pranab Sarkar, Chiranjib Majumder, “Platinum atomic wire encapsulated in gold nanotubes: A first principle study”, *AIP Conf. Proc.* 1591, 468 (2014).
19. Sandeep Nigam, Suman Kalyan Sahoo, Chiranjib Majumder, “Interaction of ammonia with semiconducting oxide surfaces”, *AIP Conf. Proc.* 1942, 120030 (2018).