

Publications/Book Chapter

Journals (SCI): Scopus Link: [Scopus-S.Sahu](#)

1. N Praveer, RK Sahoo, S Sahu, Density functional study of physisorption of H₂ molecules on scandium and yttrium decorated C₂₀ fullerene: prospect for hydrogen storage, *Journal of Molecular Modeling* 31 (1), 31(2025).
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<https://iopscience.iop.org/article/10.1088/1361-6463/ad75a1/meta>
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<https://doi.org/10.1016/j.jpcs.2023.111496>
10. Ankita Jaiswal, S. Sahu, “High capacity H₂ adsorption over Si₄Li_n (n = 1–3) binary clusters: A DFT study”, *Material Today:Proceedng*, 2023, <https://doi.org/10.1016/j.matpr.2022.12.271>
11. Labanya Bhattacharya , Alex Brown , Sagar Sharma , and S. Sahu, "Computational Design of Crescent Shaped Promising Nonfullerene Acceptors with 1,4-Dihydro-2,3-quinoxalinedione Core and Different Electron-withdrawing Terminal Units for Photovoltaic Applications" *J. Phys. Chem. A* 126, 40, 7110–7126

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22. Ankita Jaiswal, Rakesh K Sahoo, Shakti S Ray, S Sahu " Alkali metals decorated silicon clusters (Si_nM_n , $n = 6, 10$; $M = Li, Na$) as potential hydrogen storage materials: A DFT study" *International Journal of Hydrogen Energy* 46 (80), 1775-1789 (2022) doi.org/10.1016/j.ijhydene.2021.10.228
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29. G Gogoi, L Bhattacharya, Smruti R. Sahoo, S Sahu, NS Sarma, S. Sharma, "Enhancement of air-stability, pi-stacking ability, and charge transport properties of fluoroalkyl side chain engineered n-type naphthalene tetracarboxylic diimide compounds" *RSC Adv.*, 11, 57 (2020); <https://doi.org/10.1039/D0RA08345C>
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B. Proceedings (Scopus) :

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Book Chapter:

1. Hydrogen storage challenge in the hydrogen-based civilization (Hydrogen Fuel Cell Technology for Mobile Applications) ,IGI Publishing House