

Publications/Book Chapter

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

1. Rakesh K. Sahoo, and S.Sahu, "Physisorption and chemisorption hydrogen molecules on Ti functionalized [2,2,2]Paracyclophane: Insight from density functional study" *Journal of Energy Storage*, 63. (2023): 106951. <https://doi.org/10.1016/j.est.2023.106951>
2. Ankita Jaiswal, B. Chakraborty, S. Sahu, A "Computational Insight on the Effect of Encapsulation and Li Functionalization on Si₁₂C₁₂ Heterofullerene for H₂ Adsorption: A Strategy for Effective Hydrogen Storage", *ACS Appl. Energy Mater.* 6, 6, 3374 (2023) : <https://doi.org/10.1021/acsaem.2c04082>
3. Rakesh K. Sahoo, and S. Sahu, "Reversible hydrogen storage in Li functionalized [2,2,2]Paracyclophane at cryogenic to room temperatures: A computational quest" *Energy Storage*, 2023.
4. 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>
5. 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 2022, <https://doi.org/10.1021/acs.jpca.2c03906>
6. B. Chakraborty, A. Vaidyanathan, M. Kandasamy, V. Wagh, S. Sahu "High-capacity hydrogen storage in yttrium-decorated Ψ-graphene: Acumen from density functional theory" *Journal of Applied Physics* 132, 065002 (2022), <https://doi.org/10.1063/5.0098522>
7. R. K. Sahoo, S. Sahu" Reversible hydrogen storage capacity of Li and Sc doped novel C₈N₈ cage: Insights from density functional theory" *Int J Energy Res.*2022;1–16. <https://doi.org/10.1002/er.8562>
8. R Khatua, S Debata, S Sahu, ' Computational study of electron transport in halogen incorporated diindenotetracene compounds: crystal structure, charge transport and optoelectronic properties' , *Phys. Chem. Chem. Phys.* 24, 13256, 2022. DOI: [10.1039/d1cp05784g](https://doi.org/10.1039/d1cp05784g)
9. Suryakanti Debata,, Nataliya Karaush-Karmazin,, Glib Baryshnikov, and S. Sahu, "Theoretical Investigation of Charge Transport and Optoelectronic Properties of Bowl-Shaped Dicyclopenta[ghi,pqr]perylene Derivatives" *ACS Appl. Electron. Mater.* 2022, 4, 8, 4146–4159. <https://doi.org/10.1021/acsaelm.2c00778>
10. Ankita Jaiswal, B. Chakraborty, S. Sahu, "High capacity reversible hydrogen storage in Si substituted and Li decorated C₂₀ fullerene: Acumen from density functional theory simulations" *Int J Energy Res.*2022;1–17, <https://doi.org/10.1002/er.8524>

11. R. K Sahoo, B. Chakraborty, S. Sahu, 'Reversible hydrogen storage capacity of Sc and Y functionalized [1, 1] paracyclophane: Insights from density functional study. *Int. J. Hydr. Energy*. 47, 2022, 18881-18895. <https://doi.org/10.1016/j.ijhydene.2022.06.294>
12. S. S. Ray, R. K. Sahoo., S. Sahu, "Reversible hydrogen storage capacity of vanadium decorated small boron clusters (BnV2, n= 6-10): A dispersion corrected density functional study". *Comp. Theo. Chem.*, 1217, 113899,2022. <https://doi.org/10.1016/j.comptc.2022.113899>
13. Rakesh K. Sahoo, S. B. Barik, and S. Sahu, "Hydrogen Storage Capacity of Vanadium functionalized [2,2]paracyclophane: A DFT Study" . *Materials Today: Proceeding* 66, 3360-3363(2022):. <https://doi.org/10.1016/j.matpr.2022.07.125>.
14. Rakesh K. Sahoo, R. Khatua, and S. Sahu, "Theoretical study of Linear and Non-linear Optical Properties of Small CaC_n (n= 2-7) Clusters". *Materials Today: Proceeding*, 66, 3397-3400 (2022):. <https://doi.org/10.1016/j.matpr.2022.07.304>.
15. S. Debata, R. Khatua, S. Sahu, [Synergistic effects of side-functionalization and aza-substitution on the charge transport and optical properties of perylene-based organic materials: a DFT study](#), *New. J. Chem*, 46(21), pp. 10402–140414, 2022
16. 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
17. Rakesh K Sahoo, B Chakraborty, S Sahu " [Reversible hydrogen storage on alkali metal \(Li and Na\) decorated C20 fullerene: A density functional study](#)" *International Journal of Hydrogen Energy* 46 (80), 40251-40261 (2021) doi.org/10.1016/j.ijhydene.2021.09.219
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19. S. Debata, R. N Khatua, S. R. Sahoo, S. Sahu, " Rational designing and crystal structure prediction of ring-fused double-PDI compounds as n-channel organic semiconductors: A DFT study" Accepted in PCCP (RSC), 2021
20. Saroj K. Parida, Debasis Behera, S. Sahu, "A computational quantum chemical and polarizability calculations of liquid crystal 4-cyano-4-pentylbiphenyl with water molecule (H₂O)", *J. Mol. Struc.*, 1227, 129568, 2021; <https://doi.org/10.1016/j.molstruc.2020.129568>
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22. Himani Tomer , Paresh Modak , S. Sahu , Bobby Antony, "Electron induced scattering cross section for pyrrole and its isomers" *Eur. Phys. J. D*, 74: 198(2020); <https://doi.org/10.1140/epjd/e2020-10283-4>

23. 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>
24. R Khatua, Smruti R. Sahoo, S Sharma, S Sahu "Anisotropic charge transport and optoelectronic properties of wide band gap organic semiconductors based on biphenyl derivatives: A computational study" *Synthetic Metals* 267, 116474 (2020); <https://doi.org/10.1016/j.synthmet.2020.116474>
25. R Khatua, S Debata, S Sahu "Computational characterization of N-type characteristics and optoelectronic properties in air-stable pyromellitic diimide derivatives" *New Journal of Chemistry* 44 (20), 8412 (2020); <https://doi.org/10.1039/D0NJ00811G>
26. G Gogoi, L Bhattacharya, S Rahman, NS Sarma, S Sahu, BK Rajbongshi, S. Sharma "New Donor-Acceptor-Donor type of organic semiconductors based on the regioisomers of diketopyrrolopyrroles: A DFT study" *Materials Today Communications*, 101364 (2020); <https://doi.org/10.1016/j.mtcomm.2020.101364>
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29. Gautomi Gogoi, Smruti Ranjan Sahoo, Basant Kumar Rajbongshi, S. Sahu, Neelotpal Sen Sharma, Sagar Sharma, New types of organic semiconductor based on diketopyrrolopyrroles and 2,1,3-benzochalcogenadiazoles: a computational study ", *Journal of Molecular Modelling*, 25:42 (2019), <https://doi.org/10.1007/s00894-019-3922-x>
30. Shakti Sahnkar Ray, Smruti Ranjan Sahoo, and S. Sahu, Hydrogen storage in scandium doped small boron clusters (BnSc2, n=3-10): A density functional study, *International Journal of Hydrogen Energy*, 44, 5661 (2019); <https://doi.org/10.1016/j.ijhydene.2018.12.109>
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34. Saroj K. Parida, S. Sahu, "A density functional study of second-row dicarbides C₂X (X=Na-Cl) with carbon monosulfide molecule: molecular structure and bonding mechanism", *Material Research Express* (2018), 5(5), 055604/1-055604/7; <https://orcid.org/0000-0002-6784-6436>
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36. Smruti Ranjan Sahoo, S. Sahu, and Sagar Sharma, " Charge Transport, Optical, and Non-linear Optical Properties of CF₃-substituted Acene Compounds: A DFT Study ", *Theoretical Chemistry Account*, 136:99 (2017); <https://doi.org/10.1007/s00214-017-2131-x>
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38. Saroj K. Parida, S. Sahu, and Sagar Sharma, "Regioselectivity of third-row main group dicarbides, C₂X (X=K-Br) for CO interaction: Fukui function and topological analyses", *Chemical Physics Letters* (2016) 659, 216-220; <https://doi.org/10.1016/j.cplett.2016.06.053>
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B. Proceedings (Scopus) :

1. Rakesh K. Sahoo, Shakti S. Ray, and Sridhar Sahu. "A density functional study of hydrogen storage in Li decorated C 20 fullerene." AIP Conference Proceedings. 2269. (2020): 030110. <https://doi.org/10.1063/5.0019528>
2. Shakti S. Ray, Rakesh K. Sahoo, and Sridhar Sahu. "A theoretical study of non linear optical responses and photo-absorption in carbon doped boron cluster" AIP Conference Proceedings. 2269. (2020): 030111. <https://doi.org/10.1063/5.0019812>
3. Density functional study of the optoelectronic and photovoltaic properties of cyclopentadithiophene-benzothiadiazole donor-acceptor copolymer: Effect of structural modification, L Bhattacharya, S Sahu, AIP Conference Proceedings 2220 (1), 130017, (2020)
4. Smruti Ranjan Sahoo, Sridhar Sahu, and Sagar Sharma, " *Charge transport optical properties of trifluoromethyl substituted benzodithiophene (TFMBDT): A theoretical study* ", AIP conference proceedings 1953, 140008 (2018); doi: 10.1063/1.5033183.
5. Theoretical study on charge transport properties of high mobility n-channel organic semiconductor-hexachloro-hexa-azatrinaphthylene, R Khatua, S Debata, S Sahu

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6. Density functional study of the optoelectronic and photovoltaic properties of cyclopentadithiophene-benzothiadiazole donor-acceptor copolymer: Effect of structural modification, L Bhattacharya, S Sahu, AIP Conference Proceedings 2220 (1), 130017 (2020)
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8. Anisotropic charge transport in 7, 10-diphenyl-8, 9-diazafluoranthene as n-type organic semiconductor: A DFT study, R Khatua, S Sahu AIP Conference Proceedings 2100 (1), 020016 (2019)
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14. Smruti Ranjan Sahoo, Saroj Kumar Parida, and Sridhar Sahu, " *A theoretical study of charge transport properties of trifluoromethyl (-CF₃) substituted naphthalene (TFMNA) molecule* ", IOP conf. series: Material Science and Engineering, 149, 012164 (2016); doi: 10.1088/1757-899X/149/1/012164.
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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