List of Publications

Related To Thesis

1. **Darshil Chodvadiya**, Prafulla K. Jha, and Brahmananda Chakraborty. "Theoretical inspection of Ni/α-SiX (X= N, P, As, Sb, Bi) Single-Atom catalyst: Ultra-high performance for hydrogen evolution reaction." ***International Journal of Hydrogen Energy (2022)*****:** 47(99), 41733-41747.
2. **Darshil Chodvadiya**, Brahmananda Chakraborty, and Prafulla K. Jha. "Transition metal atoms anchored 2D holey graphyne for hydrogen evolution reaction: Acumen from DFT simulation." ***International Journal of Hydrogen Energy (2023)*****:** 48(48), 18326-18337.
3. **Darshil Chodvadiya**, Madhavi H. Dalsaniya, Narayan N. Som, Brahmananda Chakraborty, Dominik Kurzydłowski, Krzysztof J. Kurzydłowski, and Prafulla K. Jha. "Defects and doping engineered two-dimensional o-B_2N_2 for hydrogen evolution reaction catalyst: Insights from DFT simulation." ***International Journal of Hydrogen Energy (2023)*****:** 48(13), 5138-5151.
4. **Darshil Chodvadiya**, Shreya Kanabar, Brahmananda Chakraborty, and Prafulla K. Jha. "Exploring the hydrogen storage possibility of the pristine, defected and metals decorated o-B_2N_2 monolayers: Insights from DFT simulations." *(Submitted to Journal)*.

Other Than Thesis

1. Jay Panchal, Apeksha Gauswami, **Darshil Chodvadiya,** Harendrasinh Jadeja and Prafulla K. Jha. "Adsorption Performance of CO, NO and NH_3 Hazardous Gas Molecules over B_9N_9 and Al_9N_9 Nanoclusters: Acumen from Density Functional Theory." *(Status: Submitted to Journal).*
2. Bhautik R. Dhori, **Darshil Chodvadiya** and Prafulla K. Jha. "Evidence of topological phase transition with excellent catalytic activity in AgCaAs Heusler alloy: A first-principles investigation." ***Journal of Physical Chemistry C*** **(2023)**: 127(31), 15461–15473.
3. Paras Patel, Saurav Patel, **Darshil Chodvadiya**, Madhavi H. Dalsaniya, Dominik Kurzydłowski, Krzysztof J. Kurzydłowski, and Prafulla K. Jha. "A density functional theory study on the assessment of α-CN and α-CP monolayers as anode material in Li-ion batteries." ***Journal of Energy Storage (2023)***: 71, 108074

4. Shardul Vadalkar, **Darshil Chodvadiya**, Narayan N. Som, Keyur N. Vyas and Prafulla K. Jha. "Cyclo[18]carbon as a Hazardous Gas Scavenger: Effect of Boron and Nitrogen Doping on Molecular Adsorption." ***ChemistrySelect (2023)***: 8(23), e202204862.
5. Pratikkumar Lakhani, **Darshil Chodvadiya**, Prafulla K. Jha, Vivek Kumar Gupta, Damian Trzybiński, Krzysztof Wozniak, Krzysztof Kurzydłowski, U. K. Goutam, Himanshu Srivastava, Chetan K. Modi. "DFT stimulation and experimental insights of chiral Cu(II)-salen scaffold within the pocket of MWW-zeolite and its catalytic study." ***Physical Chemistry Chemical Physics (2023)*:** 25, 14374-14386.
6. Paras Patel, Saurav Patel, **Darshil Chodvadiya**, Madhavi H. Dalsaniya, Dominik Kurzydłowski, and Prafulla K. Jha. "Two-Dimensional α-SiX (X = N, P) Monolayers as Efficient Anode Material for Li-Ion Batteries: A First-Principles Study." ***ACS Applied Nano Materials (2023)*:** 6(3), 2103-2115**.**
7. Sourav Kanti Jana, **Darshil Chodvadiya**, Narayan N. Som, and Prafulla K. Jha. "A quantum mechanical prediction of C_{24} fullerene as a DNA nucleobase biosensor." ***Diamond and Related Materials (2022)*:** 129, 109305.
8. **Darshil Chodvadiya**, Ujjawal Jha, Piotr Śpiewak, Krzysztof J. Kurzydłowski, and Prafulla K. Jha. "Potential anodic application of 2D h-AlC for Li and Na-ions batteries." ***Applied Surface Science (2022)*:** 593, 153424.
9. Nayana Shekh, **Darshil Chodvadiya**, and Prafulla K. Jha. "Rational design of h-AlC monolayer as anode material for Mg-ion battery: A DFT study." ***Energy Storage (2022)*:** 5(3), e415.
10. Saurav Patel, Paras Patel, **Darshil Chodvadiya**, Narayan N. Som, and Prafulla K. Jha. "Adsorption performance of C_{12}, B_6N_6 and Al_6N_6 nanoclusters towards hazardous gas molecules: A DFT investigation for gas sensing and removal application." ***Journal of Molecular Liquids (2022)***: 352, 118702.
11. Shardul Vadalkar, **Darshil Chodvadiya**, Narayan N. Som, Keyur N. Vyas, Prafulla K. Jha, and Brahmananda Chakraborty. "An Ab-initio Study of the C_{18} nanocluster for Hazardous Gas Sensor Application." ***ChemistrySelect (2022)***: 7(3), e202103874.
12. **Darshil Chodvadiya**, Narayan N. Som, Prafulla K. Jha, and Brahmananda Chakraborty. "Enhancement in the catalytic activity of two-dimensional α-CN by B, Si and P doping for hydrogen evolution and oxygen evolution reactions." ***International Journal of Hydrogen Energy (2021)*:** 46(43), 22478-22498.
13. Trupti K. Gajaria, **Darshil Chodvadiya**, and Prafulla K. Jha. "Density functional theory investigation of thermal conductivity in α-CN and α-CP monolayers: Implications for

thermal management of electronic devices." ***ACS Applied Nano Materials (2021)*****:** 4(5), 4474-4483.

14. Shardul Vadalkar, **Darshil Chodvadiya**, Keyur N. Vyas, and Prafulla K. Jha. "Adsorption of HCN on pristine and Al/Si/P decorated C_{18} nanocluster: a first principles study." ***Materials Today: Proceedings (2022)***: 67, 229-237.
15. **Darshil Chodvadiya**, Prafulla K. Jha and Brahmananda Chakraborty. "Introduction of Defects in 2D α-SiN for Improvement in Hydrogen Evolution Reaction Activity: A DFT Study." ***Proceedings of the 65th DAE Solid State Physics Symposium (2021)*****:** 574-575.
16. **Darshil Chodvadiya**, Sharad Babu Pillai, Brahmananda Chakraborty, and Prafulla K. Jha. "Strain effect on Mexican-hat dispersion and electronic band gap of 2D α-CN." ***AIP Conference Proceedings (2020)*****:** 2265(1), 030377.