

List of Publication and Presentations

Publications Related to Thesis

- 1) **Heli Mistry**, Darshil Chodvadiya, Shardul Vadalkar, Keyur N. Vyas, and Prafulla K. Jha. "Interaction study of CO and NO pollutant gases with pristine, defected and doped α -CX (X= N, P) monolayers using density functional theory." *Surfaces and Interfaces* 46 (2024): 103958.
- 2) **Heli Mistry**, Bhautik R. Dhori, Maitry Joshi, Keyur N. Vyas and Prafulla K. Jha. "Hazardous CO, NO, NH₃ Gases over Boron and Beryllium Doped α -CN Monolayers: A First Principles Study for Sensing and Removal Applications". *Materials Chemistry and Physics* 327(2024): 129875
- 3) **Heli Mistry**, Shardul Vadalkar, Keyur N. Vyas, and Prafulla K. Jha. "Adsorption Mechanism of Ni Decorated α -CN Monolayer towards CO, NO, and NH₃ Gases: Insights from DFT and Semi-classical Studies." *Materials Science in Semiconductor Processing* 186 (2025): 109106
- 4) **Heli Mistry**, Darshil Chodvadiya, Shardul Vadalkar, Keyur N. Vyas, and Prafulla K. Jha. "Ammonia adsorption over Al-doped α -CN monolayer: A first principles study" (manuscript under preparation).

Publications Non-related to Thesis

- 1) Shardul Vadalkar, Darshil Chodvadiya, **Heli Mistry**, Narayan N. Som, Keyur N. Vyas, and Prafulla K. Jha. "Toxic gas removal using transition metal-decorated Cyclo [18] carbon: A first principles prevision." *Computational and Theoretical Chemistry* 1238 (2024): 114724.
- 2) Shardul Vadalkar, **Heli Mistry**, Narayan N. Som, and Prafulla K. Jha. "Enhancing Hydrogen Evolution Activity of α -CP Monolayer through P-block Doping: A DFT Study" (manuscript under preparation)

Presentation:

1. Poster presentation entitled "Adsorption Performance of NO gas molecule over pristine and doped α -CN Monolayer: A DFT study" in 66th DAE Solid State Physics Symposium- BIT Mesra (December-2022)
2. Poster presentation entitled "Adsorption performance of CO gas molecule over pristine and doped α -CN Monolayer: A DFT study" in *Advances in Materials Science: Challenges and Opportunities*- Bhavnagar (March-2023)