

# List of Publications

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## Publications related to Thesis

1. **Shardul Vadalkar**, Darshil Chodvadiya, Narayan N. Som, Keyur N. Vyas, Prafulla K. Jha, and Brahmananda Chakraborty. "An Ab-initio Study of the C<sub>18</sub> Nanocluster for Hazardous Gas Sensor Application." *ChemistrySelect* **7**, no. 3, e202103874 (2022).
2. **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* **8**, no. 23, e202204862 (2023).
3. **Shardul Vadalkar**, Darshil Chodvadiya, Heli Mistry, Narayan Som, Keyur N. Vyas, and Prafulla K. Jha. "A First Principles Prediction of Transition Metal-decorated Cyclo[18]carbon as a Toxic Gas Scavenger: Study of Structural, Electronic, Topological, and Spectroscopic Properties" (Submitted).
4. **Shardul Vadalkar**, Darshil Chodvadiya, Keyur N. Vyas, and Prafulla K. Jha. "Adsorption of HCN on Pristine and Al/Si/P Decorated C<sub>18</sub> Nanocluster: A First Principles Study." *Materials Today: Proceedings* **67**, 229-237 (2022). (Conference proceeding publication)

## Publications non-related to Thesis

1. Kanzariya, Ashvin, **Shardul Vadalkar**, Sourav Kanti Jana, L. K. Saini, and Prafulla K. Jha. "An ab-initio investigation of transition metal-doped graphene quantum dots for the adsorption of hazardous CO<sub>2</sub>, H<sub>2</sub>S, HCN, and CNCl molecules." *Journal of Physics and Chemistry of Solids*, 111799 (2023).
2. Heli Mistry, Darshil Chodvadiya, **Shardul Vadalkar**, Keyur N. Vyas, and Prafulla K. Jha. "Interaction Study of Pollutant CO and NO Gases with Pristine, Defected and Doped  $\alpha$ -CX (X = N, P) Monolayers using Density Functional Theory" (Submitted).
3. Kanzariya, Ashvin, **Shardul Vadalkar**, L. K. Saini, and Prafulla K. Jha. "Cyclo[16]carbon through the Lens of Density Functional Theory: Effect of Impurity Decoration on Hydrogen Evolution Reaction." (Submitted)