Published Articles/Papers in Journals: Related to Thesis

1. Basant Roondhe, Shweta D. Dabhi and Prafulla K. Jha "Sensing properties of pristine boron nitride nanostructures towards alkaloids: A first principles dispersion corrected study" *Applied Surface Science* **441**, 588 (2018), DOI: 10.1016/j.apsusc.2018.01.249.
2. Basant Roondhe and Prafulla K. Jha, ""Haeckelite" a new low dimensional member of boron nitride family for Biosensing with ultra-fast recovery time: A first principles investigation" *Journal of Materials Chemistry B* **6**, 6796 (2018), DOI: 10.1039/C8TB01649F
3. Basant Roondhe and Prafulla K. Jha, "Neurotransmitter-Functionalized Boron Nitride Nanoribbons as Biological Cargo Carriers: Analysis by Density Functional Theory" *ACS Applied Nano Materials* **2**, 1552 (2019). DOI:10.1021/acsanm.9b00028.

Published Articles/Papers in Journals: Not Related to Thesis

1. Basant Roondhe, Prafulla K Jha, Rajeev Ahuja, "Haeckelite boron nitride as nano sensor for the detection of hazardous methyl mercury" *Applied Surface Science* **496**, 143685 (2019). https://doi.org/10.1016/j.apsusc.2019.144860.
2. Khushbu Patel, Bhumi A. Baraiya, Narayan N. Som, Basant Roondhe and Prafulla K. Jha, "Investigating Hydrogen Evolution Reaction Properties of a New AlC Honeycomb 2D" *Int. J. Hydrog. Energy* (*Accepted*) (2019). https://doi.org/10.1016/j.ijhydene.2019.10.131.

3. Trupti K. Gajaria, Basant Roondhe, Shweta D. Dabhi and Prafulla K. Jha, "Exploring the Hidden Catalyst from Boron Pnictide Family for HER and OER" *Int. J. Hydrog. Energy* (*Accepted*) (2019). https://doi.org/10.1016/j.ijhydene.2019.09.107.

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5. Basant Roondhe, Khushbu Patel and Prafulla K. Jha, "Two-Dimensional Metal Carbide Comrade for Tracing CO and CO_2" *Applied Surface Science* **496**, 143685 (2019). https://doi.org/10.1016/j.apsusc.2019.143685.

6. Deepak Upadhyay, Basant Roondhe, Arun Pratap and Prafulla K. Jha, "Two-dimensional delafossite cobalt oxyhydroxide as a toxic gas sensor" *Applied Surface Science* **476**, 198 (2019), DOI: 10.1016/j.apsusc.2019.01.057

7. Khushboo Patel, Basant Roondhe, Shweta D. Dabhi and Prafulla K. Jha, "A new flatland buddy as toxic gas scavenger: a first principles study" *Journal of Hazardous Materials* **351**, 337 (2018), DOI: 10.1016/j.jhazmat.2018.03.006

8. Shweta D. Dabhi, Basant Roondhe and Prafulla K. Jha, "Nucleobases Decorated Boron Nitride Nanoribbon for Electrochemical Bio-sensing: A Dispersion Corrected DFT Study" *Physical Chemistry Chemical Physics* **20**, 8943 (2018), DOI: 10.1039/C7CP08145F

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