List of publication related to thesis

- **Bhumi A. Baraiya**, Hemang Tanna, Venu Mankad, and Prafulla K. Jha, Dressing of Cu Atom over Nickel Cluster Stimulating the Poisoning-Free CO Oxidation: An Ab Initio Study, The Journal of Physical Chemistry A, **125**, 5256-5272, (2021). DOI: /10.1021/acs.jpca.1c02354.

- **Bhumi A. Baraiya**, Venu Mankad, Prafulla K. Jha, Uncovering the structural, electronic and vibrational properties of atomically precise Pd_mCu_n clusters and their interaction with CO_2 molecule, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, **229**, 117912, (2020). **DOI:** 10.1016/j.saa.2019.117912.

- **Bhumi A. Baraiya**, Venu Mankad, Prafulla K. Jha, CO_2 hydrogenation to Methanol, Formic acid and Methane over Pd_5Cu_8 cluster: A First-principles Study. (To be submitted)

- **Bhumi A. Baraiya**, Venu Mankad, Prafulla K. Jha, Determining the CO Oxidation Activity of Supported Pt_3M Clusters from Frontier Orbitals. (To be submitted)

- **Bhumi A. Baraiya**, Venu Mankad, Prafulla K Jha, Degrading CO poisoning over foreign atom seized $Ag_{12}M$ icosahedral bimetallic clusters, AIP Conference Proceedings, **2265**, 030612, (2020). DOI: 10.1063/5.0016620.

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