



I joined Prof. Lapkin's group in 2019 as an MPhil student after completing my B.tech in Chemical engineering at the Indian Institute of Technology, Roorkee. Currently I am continuing my PhD under his supervision under the Syntech CDT program.

I joined Syntech CDT program with Chemistry department as part of my PhD in October 2020. This program has offered me with so many preparatory courses required in my research, with added assessments and feedback from experts in different research areas.

My research aims to develop a generalized catalyst design scheme for gas phase heterogeneous reaction, specifically focusing on reaction involving Carbon Capture and fuel generation, e.g. CO₂ methane reforming, CO₂ methanation, etc. My research uses Material databases to train machine learning models for predicting reaction energies for catalyst optimization for a particular reaction system.

Publications

1. Chopra, U., et al., *Accurate and general formalism for spin-mixing parameter calculations*. Physical Review B, 2019. **100**(13): p. 134410.
2. Chopra, U., et al., *First-principles study of thermoelectric properties of Li-based Nowotony–Juza phases*. Journal of Physics: Condensed Matter, 2019. **31**(50): p. 505504.