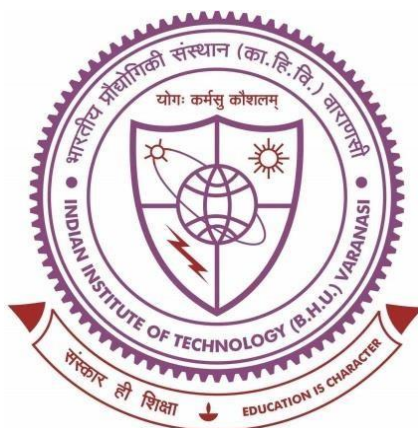


**Conformational landscape and metal-molecule
interaction of diverse molecular systems:
Insights from *ab initio* electronic structure
calculations**



**THESIS SUBMITTED IN PARTIAL FULFILLMENT
FOR THE AWARD OF DEGREE**

DOCTOR OF PHILOSOPHY

By

POONAM BHADORIA

**Department of Chemistry
Indian Institute of Technology
(Banaras Hindu University), Varanasi**

Roll No. 18051001

Year 2023