INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

Name of the Student	:	Kushagra Agrawal
Roll Number	:	166107102
Programme of Study	:	Ph.D.

Thesis Title: HYDRODEOXYGENATION OF BIO-OIL MODEL COMPOUNDS IN SOLVENTS AND OVER CARBON-BASED CATALYST USING DENSITY FUNCTIONAL THEORY

Name of Thesis Supervisor(s)	:	Prof. Nanda Kishore
Thesis Submitted to the Department/ Center	:	Chemical Engineering
Date of completion of Thesis Viva-Voce Exam	:	20th August 2021
Key words for description of Thesis Work	:	Biomass; Hydrodeoxygenation; DFT; solvent; Molybdenum Carbide

---

SHORT ABSTRACT

In this dissertation, the hydrodeoxygenation of bio-oil model compounds like xylose, dibenzofuran, guaiacol and formic acid is studied in the solvent environment, as well as over carbon-based catalyst using the density functional theory. First, the upgrading of xylose is studied using B3LYP and M06-2X functional to establish a comparison between the two functionals for thermochemistry calculations. For incorporating the solvation effect, an implicit solvation model – SMD, was used. Next, the upgrading of dibenzofuran is studied in the gas phase, in water solvent and in methanol solvent. The reaction scheme converting dibenzofuran to benzene and cyclohexane was proposed and the thermochemistry was calculated for the proposed mechanism. Further, the upgrading of guaiacol is also studies in an implicit water solvent environment to produce benzene, toluene and o-cresol via important intermediates like phenol and anisole. The subsequent chapter highlights the adsorption characteristics of guaiacol and phenol over nitrogen doped graphene. Non-defective and defective graphene sheets were considered for this study, and the adsorption is conducted for different orientations and arrangements of the adsorbate. Finally, the kinetics and thermochemistry of the upgrading of formic acid and guaiacol is studied over β-Mo_2C (100) surface to gain insight into the HDO mechanism of carboxylic group and phenols present in the crude bio-oil.

It is found that both B3LYP and M06-2X are equally good/bad in predicting the thermochemistry of the system of interest. Xylose hydrodeoxygenation showed that saturation of furan ring is most favourable reaction in the entire reaction scheme, and the presence of solvent improved the thermochemistry when compared to the gas phase. Dibenzofuran also showed similar trends where the presence of water solvent was found to be most suitable medium over methanol and gas phase, and the conversion to cyclohexane was preferred. The guaiacol upgrading showed formation of benzene to be thermochemically most favourable upgraded product, and solvent environment to be equal or better than gas phase. In the adsorption of phenol and guaiacol over nitrogen doped graphene, it was observed that the presence of nitrogen increased the adsorption energy, when compared to pristine graphene by more than double. Upgrading studies of HCOOH and guaiacol over molybdenum carbide show that the surface is susceptible to poisoning by carbon containing species like CO and CH_2 due to high carburization potential.