# SECOND SEMESTER 2020-21 COURSE HANDOUT

Date: 15.01.2021

In addition to part I (General Handout for all courses appended to the Time table) this portion gives further specific details regarding the course.

Course No : CHEM F 431

Course Title : Sustainable Chemistry using Renewables

Instructor-in-Charge: Bibhas R. Sarkar

Instructor(s) : -Tutorial/Practical Instructors: --

1. Course Description: The course will provide an overview of the chemistry involved with the utilization of renewable resources as alternative feedstock for the chemicals and fuels industry, to the currently used ones. Major emphasis is focused on the chemistry of the renewable bio-based alternative resources and understanding of their potential as feedstock of future, within the mainstream process structure, to visualize viable switch-over as necessary. The course will encompass around the bio-refinery concept and will describe the chemistry in all the essential branches of renewable resources (biomass, oils/ fats, H<sub>2</sub>, CO<sub>2</sub> etc.) and will proliferate the practicality aspect of applied chemistry using catalysis approach for sustainable technology development.

# 2. Scope and Objective of the Course:

The course will be broadly divided into broad topics as in the course plan. Learning objectives for each of these broad topics as discussed in the course plan has been described in terms of the projected outcomes – what the learner should be able to do by studying these.

- 3. Text Books: Catalysis for Renewables by G. Centi and R. A. van Santen (Eds), Wiley-VCH, 2007
- **4. Reference Books:** Green Carbon Dioxide: Advances in CO<sub>2</sub> Utilization by G. Centi and S. Perathoner (Eds.) Wiley, 2014

#### 5. Course Plan:

| Module | Lecture Session                        | Reference   | Learning outcomes                                 |
|--------|--|-------------|---|
| No.    |  |             |   |
| 1      | 1.1: Renewables chemistry and          | T1: 1.1-1.5 | (i) Describe the advantages and disadvantages     |
|        | catalysis, (L01-L02)                   |             | of the current technological scenario with        |
|        | <u>Topics</u> : Introduction, Economic |             | respect to the economic and societal concerns,    |
|        | and societal concerns of               |             | (ii) Discuss the alternative technology options   |
|        | conventional petro-based               |             | using renewable resources as feedstock for        |
|        | technology , Alternative               |             | chemical industry                                 |
|        | technology options, Process            |             |   |
|        | options using biomass                  |             |   |
|        | 1.2: Chemicals from renewable          | T1: 3.1-3.6 |   |
|        | resources, (L03-L07)                   |             | (i) Specify the basic facets of the bio-refinery  |
|        | Topics: Bio-refinery concept,          |             | concept, (ii) State the different strategies for  |
|        | Strategies for biomass utilization,    |             | the effective utilization of biomass as           |
|        | Platform molecules, Degraded           |             | renewable resource, (iii) Define and describe     |
|        | molecules, Biomass conversions         |             | different platform and degraded molecules, (iv)   |
|        | by new catalytic synthesis routes,     |             | Cite catalytic routes, cascade reactions, one-pot |
|        | Catalytic cascade reactions, One-      |             | reaction strategies for the use of renewable      |
|        | pot multi-product synthesis            |             | resources   |
| 2      | 2.1: Chemistry in lignocellulose       | T1: 2.1-2.6 | (i) Describe the various biomass resources with   |
|        | conversions, (L08-L12)                 |             | respect to composition etc., (ii) State and       |
|        | <u>Topics:</u> Need for biomass        |             | discuss chemistry for the different conversion    |
|        | resources, composition, Chemistry      |             | processes as, using carbohydrates, pyrolysis,     |



# BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE, Pilani Pilani Campus AUGS/ AGSR Division

| भीनं परमं बर्ट |  |                          |   |
|----------------|--|--------------------------|---|
|                | and processes for (i) using carbohydrates, (ii) Pyrolysis, (iii) Gasification, (iv) Hydrolysis, (v) Sugar derivatives; Economics associated therewith  |                          | gasification, hydrolysis etc. and many others   |
| 3              | 3.1: Bio-based Oleochemicals, (L13-L17)  Topics: Raw material scenario, Ecological compatibility, Products and applications (Polymers, dimer acids, polyols based on epoxides, fatty acids based lubes and surfactants, amino acids, carbohydrate-based surfactants, Esters, Guerbet alcohols etc.)  | T1: 4.1-4.5              | (i) Describe the raw-material situation for use of natural fats/ oils as renewable feedstock for chemicals, (ii) State the products base and applications for the bio-based oleochemicals, (iii) Chemistry strategies for polymers, acids, polyols, surfactants, esters etc.  |
|                | 3.2: Fatty acid epoxidation, (L18-L21)  Topics: Non-catalytic, Catalytic and Chemo-enzymatic epoxidation of fatty acids, Epoxidation of FAMEs (pure, mixtures, oilderivatives etc.)  | T1: 12.1-12.6            | (i) Study of scope of catalytic epoxidation chemistry as sustainable technology, (ii)  Describe the chemistry of epoxidation reactions with respect to mechanism specific to the catalytic/ non-catalytic/ enzymatic processes, (iii) describe epoxidation of FAMEs as renewable feedstock based process and other application horizons                       |
| 4              | 4.1: Fine Chemicals from renewables, (L22-L25)  Topics: Catalytic process routes for fine chemicals from bio-based molecules, case studies and examples  | T1: 5.1-5.9              | (i) Describe the chemistry involved in catalytic routes for fine chemicals arising from bio-based renewable resources, (ii) Cite case studies and discuss future directions   |
|                | 4.2: Thermochemical conversion to fuels and other chemicals, (L26-L27)  Topics: Thermal/ Thermochemical processes for fuels and other chemicals, Gasification (biomass and pyrolysis oils, fluid assisted gasification), Liquefaction process and chemistry, upgradation process and chemistry of pyrolysis oils, Catalyst design approaches, fuels from biomass | T1: 6.1-6.10,<br>7.1-7.6 | (i) Describe the chemistry of thermal and thermochemical processes for fuels and chemicals from renewable platforms, (ii) State and discuss the chemistry involved in thermal processes such as gasification, liquefaction, upgradation etc., (iv) Describe the roles of catalyst and its design chemistry with respect to thermal/ thermo-chemical processes |
| 5              | 5.1: Analyticals in thermal biomass conversions, (L28-L29)  Topics: Tunable diode laser measurement of kinetics,  Propagation of thermal fronts, influencing parameters  | T1:8.1-8.5               | (i) Describe the important analytical tools and predictive techniques for the processes using renewable resources as feedstock for chemicals  |



# BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE, Pilani Pilani Campus AUGS/ AGSR Division

| 6 | 6.1: Bio-ethanol: production, upgradation and valorization, (L30-L32)  Topics: Using bioethanol as fuel, fuel-additive, fuel blends, bioethanol and fuel cells, bio-ethanol upgradation, conversion to fuel components, conversion to other chemicals   | T1: 9.1-9.5                               | (i) Describe chemistry of utilization of bioethanol from perspective of current product diversity; (ii) Delineate the prospective/emerging process routes to other chemicals/intermediates staring from bio-based ethanol.   |
|---|---|---|--|
|   | 6.2: Glycerol as feedstock, (L33-L36)  Topics: Properties, Glycerol to fuels and additives, Etherification reaction (catalysis and kinetics), Biodiesel process and improvements, glycerol reforming (APR, steam).  Catalytic dehydration process, Oligomerization, reactions with alkenes, Catalytic oxidations, Catalytic hydrogenolysis and other miscellaneous chemistry involving glycerol | T1: 10.2-10.6;<br>11.2-11.7               | (i) State and discuss the properties and possibilities of glycerol as alternative feedstock for chemicals, (ii) Describe the modes of using glycerol and its derivatives as platforms to different chemicals/ intermediates, (iii) Cite glycerol-based catalytic processes such as dehydration, oligomerization, oxidations, hydrogenolysis, reforming etc. and discuss the chemistry associated in each |
| 7 | <b>7.1:</b> Hydrogen and CO <sub>2</sub> , (L37-L41) <u>Topics:</u> Hydrogen energy chain, H <sub>2</sub> production for alternate feedstock, , Electro-catalysis, Solar photo-catalysis, Fuel cell technology and challenges, CO <sub>2</sub> capture and valorization   | T1: 14.2-14.4;<br>16.2-16.4<br>R1: Ch 2-5 | (i) Describe the current scenario of using $H_2$ and $CO_2$ as renewable feedstock, (ii) State and discuss the existing technical knowhow on electrocatalysis, solar-photocatalysis, fuel cells etc. for production of $H_2$ , and the challenges therein (iii) Describe different strategies and process routes for utilization of $CO_2$ and the chemistry associated.                                 |

### **6. Evaluation Scheme**:

| Component             | Duration | Weightage | Date & Time       | Nature of component     |
|-----------------------|----------|-----------|-------------------|-------------------------|
|                       |          | (%)       |                   | (Close Book/ Open Book) |
| Mid-Semester Test     | 90 Min.  | 30        | <test_1></test_1> | Online tests            |
| Comprehensive         | 2 h      | 40        | <test_c></test_c> | Online tests            |
| Examination           |          |           |                   |                         |
| Continuous Evaluation | 15 min   | 30        | To be announced   | Online tests            |
|                       | each     |           |                   |                         |
|                       |          |           |                   |                         |
|                       |          |           |                   |                         |

- 7. Chamber Consultation Hour: To be announced
- **8. Notices:** All notices regarding the course will be displayed in Nalanda and/ or Department of Chemistry Notice board.
- 9. Make-up Policy: Make up would be considered only for genuine reasons
- 10. Note (if any):

Instructor-in-charge Course No. CHEM F431