INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF CENTRE: Centre for Sustainable Energy

Subject Code: SEC-503 **Course Title:** Theory and Simulation for Chemical Reactions

L-T-P: 3-0-2 **Credits:** 4 **Subject Area:** PCC

Course Outline: Key aspects of potential energy surfaces, methods for geometry optimization, identification of transition states and reaction pathways, rate constants, and transition state theory. Computational examples in homogeneous and heterogeneous catalysis, including catalytic reaction screening. Topics on basis sets, Hartree-Fock theory, correlated ab initio approaches, configuration interaction, MP2 theory, coupled-cluster techniques, multi-reference methods, density functional theory, and semiempirical approaches.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF CENTRE: Centre for Sustainable Energy

Subject Code: SEC-505 **Course Title:** Energy Conversion Technologies

L-T-P: 3-0-2 **Credits:** 4 **Subject Area:** PCC

Course Outline: Electromechanical and Electrochemical Energy Conversion systems, Wind Energy Conversion System, Solar Energy Conversion System, Hydrogen-based Energy Conversion System, conversion: Different methods of Waste to Energy, Energy production from organic wastes, Waste Energy production from plastic wastes.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF CENTRE: Centre for Sustainable Energy

Subject Code: SEC-507 **Course Title:** Energy Storage Technologies

L-T-P: 3-0-2 **Credits:** 4 **Subject Area:** PCC

Course Outline: Storage mechanisms, thermodynamic principles, Thermal energy storage - inorganic and organic phase change materials, Mechanical energy storage, Hydrogen storage - thermal decomposition of water to produce hydrogen, storage of hydrogens as protons in solid, metal hydrides, Electrochemical energy storage - charging and discharging of batteries, cyclic behaviour, introduction of lithium and sodium batteries, Supercapacitors, Fuel cells.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF CENTRE: Centre for Sustainable Energy

Subject Code: SES-501 **Course Title:** Sustainable Energy: Challenges and Industrial Perspective

L-T-P: 2-0-0 **Credits:** 2 **Subject Area:** SSC

Course Outline: Importance of energy, conventional energy sources, renewable/green energy, sources of renewable energy, energy future; Sustainability theory and practice, including population, global change, ecosystem degradation and resource limitations; Present status of renewable energy; Global warming and the forecast for humans' impact on earth's climate; Key challenges and pathways to sustainable development; Industry outlook.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF CENTRE: Centre for Sustainable Energy

Subject Code: SES-502 **Course Title:** Sustainable Transition and Policy

L-T-P: 2-0-0 **Credits:** 2 **Subject Area:** SSC

Course Outline: Energy Data and Energy Balance, accounting framework, Ratios: GDP intensity, emission intensity, Decoupling of emissions, Business of Energy, Business organization, Vertical integration, Competition amongst carriers and fuels, Fuel mixes across jurisdictions, National energy strategies, Energy Demand Analysis, Demand Management, and Demand Response, Economic analysis of Energy Investments, Challenges and Opportunities facing the energy sector.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF CENTRE: Centre for Sustainable Energy

Subject Code: SES-503 **Course Title:** Energy Economics, Policy and Planning

L-T-P: 2-0-0 **Credits:** 2 **Subject Area:** SSC

Course Outline: Energy Data and Energy Balance, accounting framework, Ratios: GDP intensity, emission intensity, Decoupling of emissions, Business of Energy, Business organization, Vertical integration, Competition amongst carriers and fuels, Fuel mixes across jurisdictions, National energy strategies, Energy Demand Analysis, Demand Management, and Demand Response, Economic analysis of Energy Investments, Challenges and Opportunities facing the energy sector.