

The Future of Chemical Technology: Integrating Biorefineries and Advanced Molecular Modeling

Key Technologies for Sustainable Development

Izabela Czekaj

Head of the group " Design of materials and catalytic processes in biorefineries and alternative fuels"
Cracow University of Technology | Faculty of Chemical Engineering and Technology
Department of Organic Chemistry and Technology (C-2)
ul. Warszawska 24, 31-155 Kraków
tel. +48 12 628 21 11, izabela.czekaj@pk.edu.pl

ABSTRACT

This lecture explores the future of chemical technology through the integration of biorefineries and advanced molecular modeling. It covers the electronic structure of lignocellulose, nano-design of zeolite-based catalysts for selective biomass conversion into chemicals, and the technological aspects of catalytic biomass valorization to carboxylic acids. Additionally, it addresses innovative catalysts for biomass gasification and methanation, selective catalytic reduction of NO_x using urea, methane combustion with a focus on Pd-PdO transformations, and the design of materials for hydrogen storage. These topics highlight the crucial role of advanced modeling in enhancing complex processes and its growing importance in future technologies.