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The Wolfson Department of Chemical Engineering

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# Rational Nanoscale Engineering of Thermocatalytic Materials for Sustainable Transformation of $CO_2$ into Renewable Synthetic Fuels

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Thermocatalytic treatment of $CO_2$-rich feedstocks (e.g., biogas, landfill gas, industrial flue gases) is an attractive route for generating Renewable Synthetic Fuels. To make the process of thermocatalytic conversion sustainable, hydrogen ($H_2$), which is required for $CO_2$ hydrogenation, should have a negligible carbon footprint. This requirement is achievable when $H_2$ is generated using renewable power (e.g., by water electrolysis). Process development starts with selecting a suitable catalytic formulation, which can be assisted by density function theory (DFT) calculations and machine learning (ML). Once selected, a synthesis method needs to be developed to create the required composition and morphology in a controllable way. Next, transport limitations must be considered at both the micro- and macro-scale. Ultimately, a conversion device (chemical reactor) needs to be designed and integrated into the $CO_2$ conversion process, which must be assessed for techno-economic feasibility. This talk focuses on the catalyst development, first outlining computational aspects and then discussing the reverse microemulsion system as a synthesis method. Aspects of reactor design, system integration and techno-economic evaluation are briefly outlined as well. Future perspectives are also discussed.