



Environmental Science journals

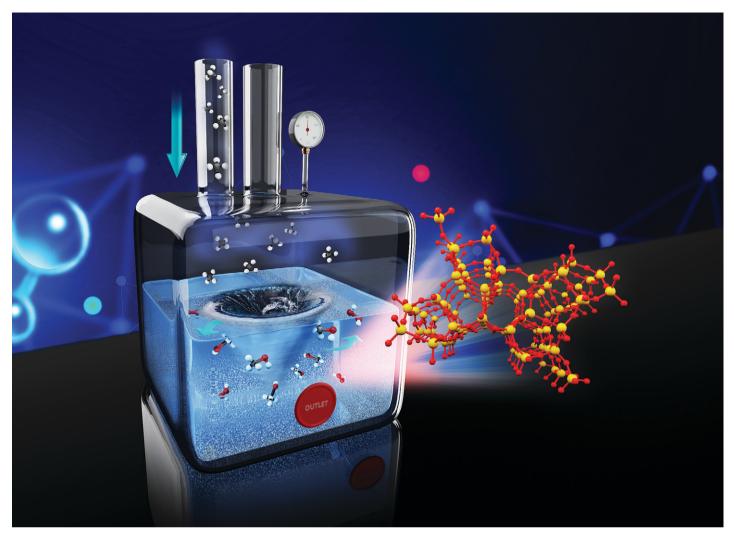
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Fundamental questions Elemental answers





Showcasing research from the Computational Catalysis group led by Dr. Jithin John Varghese, Department of Chemical Engineering, Indian Institute of Technology, Madras.

Impact of solvent sulfolane in enhancing methanol selectivity during methane partial oxidation on Fe-ZSM5 catalyst with H_2O_2 as an oxidant

The effect of sulfolane solvent in determining activity and product distribution during partial oxidation of methane to methanol using hydrogen peroxide oxidant in Fe-ZSM-5 catalyst is unravelled using a combination of Density Functional Theory and Molecular Dynamics simulations.

