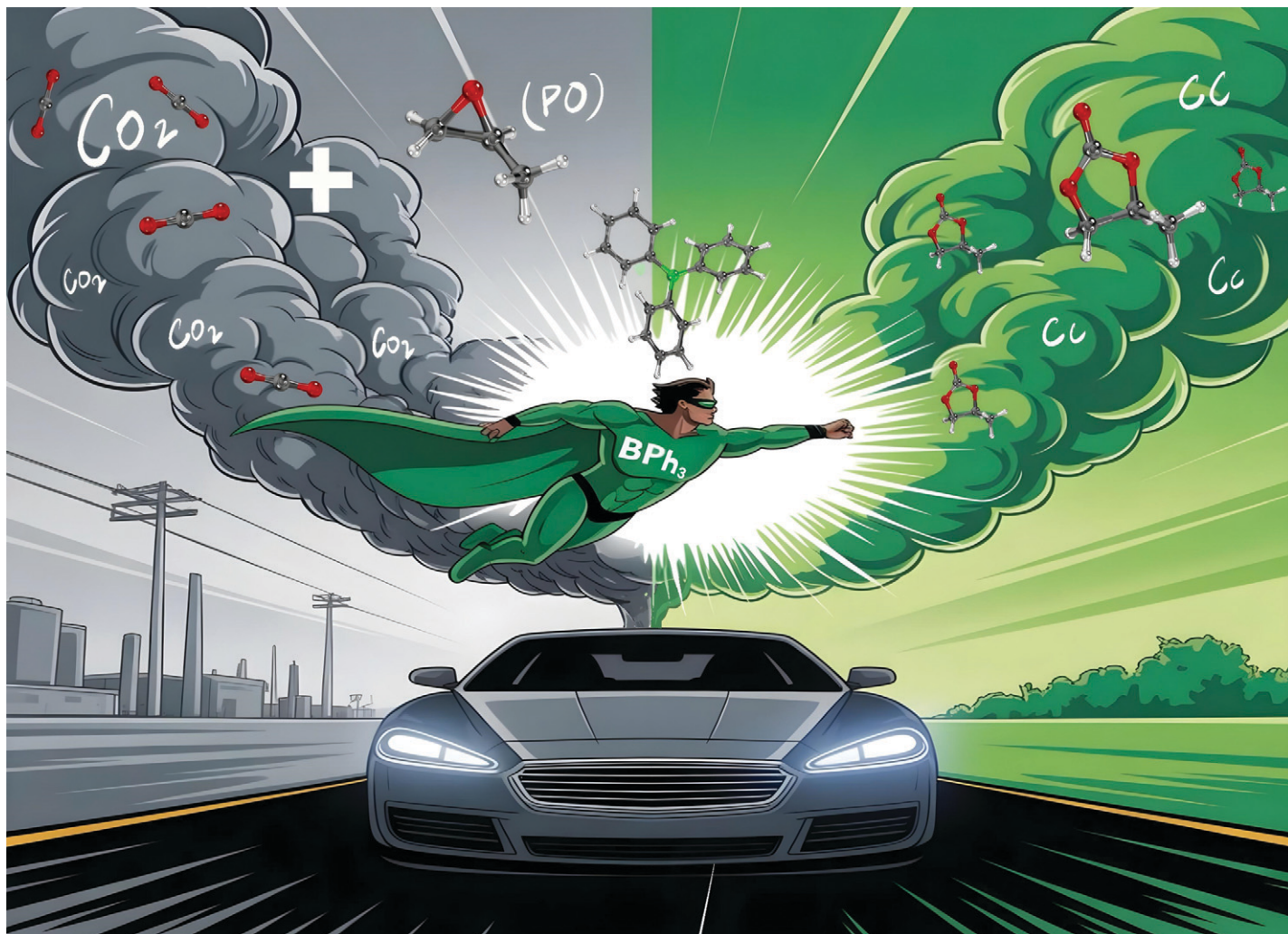




Showcasing the research work of Nikunj Kumar and Prof. Puneet Gupta at Computational Catalysis Center, Department of Chemistry, Indian Institute of Technology Roorkee, Uttarakhand, India.

Mapping the catalytic landscape of triphenylborane (BPh_3)-catalyzed CO_2 -epoxide coupling to carbonates: an *in silico* approach to solve substrate-dependent selectivity

This study explores the triphenylborane (BPh_3)-catalyzed coupling of CO_2 with epoxides, a reaction yielding either cyclic carbonates or polycarbonates depending on the substrate. Using density functional theory (DFT), the catalytic landscape is mapped to uncover the origin of substrate-dependent selectivity and identify the key steps and interactions that govern product formation.

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See Nikunj Kumar and Puneet Gupta, *Catal. Sci. Technol.*, 2025, **15**, 4661.