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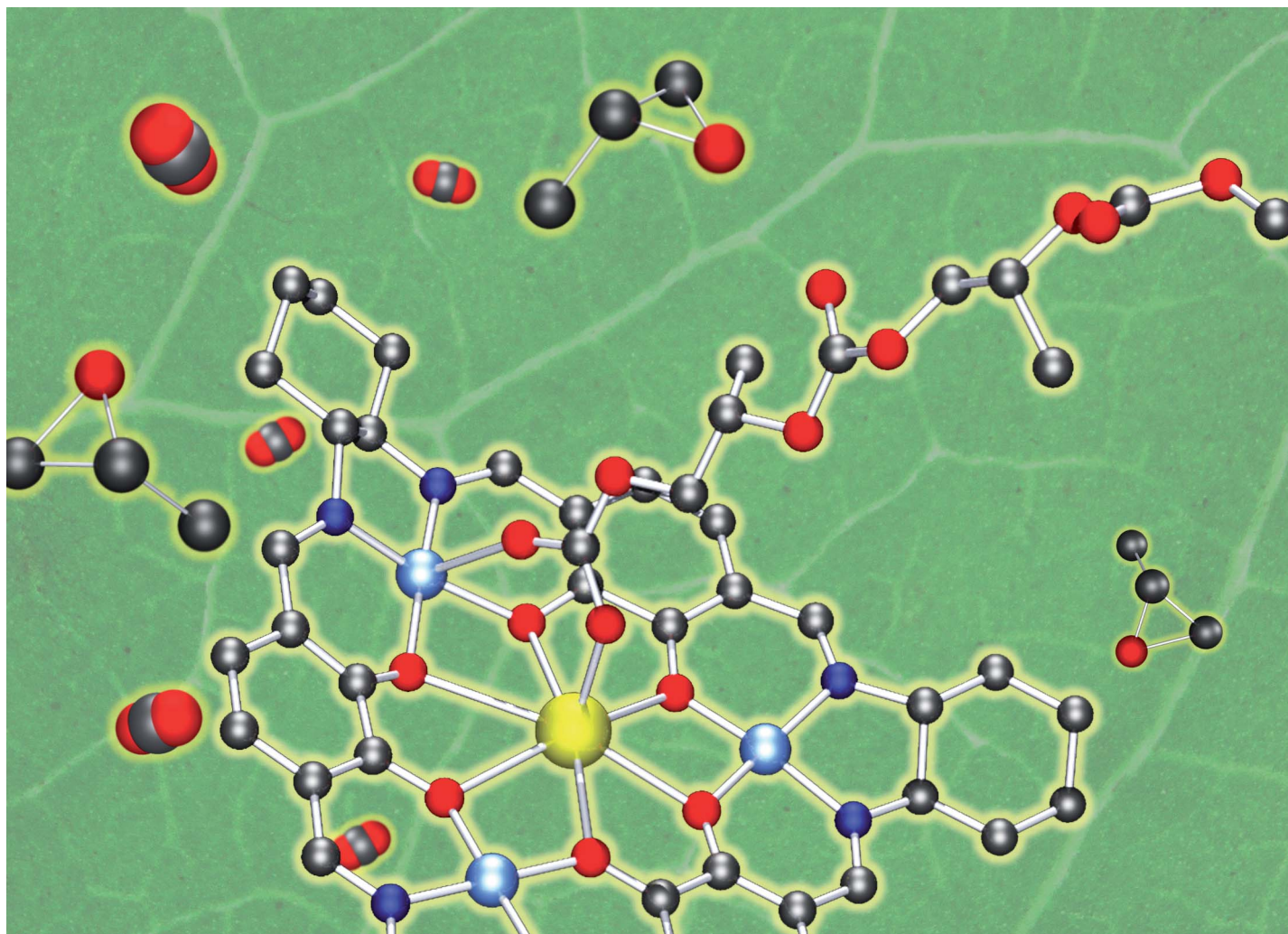
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Showcasing research from Professor Mashima's laboratory, Department of Chemistry, Graduate School of Engineering Science Osaka University.

Cationic tetranuclear macrocyclic CaCO_3 complexes as highly active catalysts for alternating copolymerization of propylene oxide and carbon dioxide

A cationic CaCO_3 hetero tetranuclear complex exhibited catalytic activity toward alternating copolymerization of propylene oxide (PO) and carbon dioxide (CO_2). The tertiary anilinium salt $[\text{PhNMe}_2\text{H}][\text{B}(\text{C}_6\text{F}_5)_4]^-$ was the best additive to generate cationic species while maintaining polymer selectivity and carbonate linkage, even under 1.0 MPa CO_2 . Density functional theory calculations clarified that the reaction pathway mediated by the cationic complex is more favorable than that mediated by the neutral complex by 1.0 kcal/mol.

As featured in:



See Jun Okuda, Kazushi Mashima *et al.*, *Chem. Sci.*, 2023, **14**, 8262.