Mechanochemically induced interfacial electronic modulation in MnCe/$BaTiO_3$ for synergistic catalysis for NO_x and o-dichlorobenzene

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Abstract

The synergistic removal of NO and chlorinated volatile organic compounds (CVOCs) using bifunctional catalysts has emerged as a cutting-edge strategy in environmental catalysis. However, achieving both efficient NOx selective catalytic reduction and CVOCs catalytic oxidation remains fundamentally challenging due to the inherent trade-off between activity and selectivity. Herein, we demonstrate that this trade-off can be overcome by applying a mechanochemical strategy coupled with electronic band modulation to construct a novel heterojunction catalyst, in which MnCe oxides are integrated with piezoelectric $BaTiO_3$ to form a heterojunction interface. The optimized TB-MnCe catalyst exhibits remarkable synergistic performance, achieving the synergistic removal of o-dichlorobenzene (>80%) and NOx (100%) within a broad temperature range of 250–350 °C. Combined experimental and theoretical investigations reveal an interfacial charge transfer of approximately 4.6 electrons from $BaTiO_3$ to MnCe during mechanochemical treatment. This charge redistribution, mediated by the engineered interface, significantly enhances the redox capability of the active sites and promotes cooperative reactions. This work highlights that atomic-level interfacial electronic modulation induced by mechanochemical processing provides a powerful route to resolve the activity-selectivity dilemma in bifunctional catalysis.

Graphical abstract