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Modelling Selective Catalytic Reduction (SCR) of NOx to N2 over Cu-SSZ-13

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Reduction of NO_x emissions from diesel engine exhaust is an environmental issue driven by increasingly stringent emission regulations. Cu-SSZ-13 catalysts have been shown to be promising for this application due to their hydrothermal stability and selectivity in reducing NO_x to N_2 using NH_3 compared to other zeolite catalysts. SO_x formed from the combustion of ppm levels of sulfur in diesel fuel deactivates the Cu-SSZ-13 catalyst. However, its effect on Cu^{2+} and CuOH active sites and the SCR mechanism is unclear and under debate