

Theoretical understanding of palladium catalysts for NO_x storage during the cold start period of vehicles

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A three-way catalytic converter (TWC) is installed in every vehicle's exhaust system to reduce the emissions of NO_x, CO, and other incompletely burned hydrocarbons, but its performance is strongly limited at low temperature. To comply with more stringent environmental regulations, reducing the emissions during the cold start period of vehicles is critical. In this study, we explore the possibility of using metallic palladium to capture NO_x and CO molecules via adsorption at low temperature ($T < 200$ °C), and release them via desorption at high temperature ($T > 200$ °C) under which TWC becomes fully operational. Computational methods such as density functional theory (DFT) and adsorbate-adsorbate interactions considered microkinetic modeling (MKM) are employed to investigate the reaction energetics and kinetics on Pd(111) and Pd(211) under different reaction conditions.