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Remarkable SO_2 and H_2S Resistant Ability on CO Oxidation by Unique Pd/WO_3 3D Hollow Sphere Nanocatalyst: Correlating Structure–Activity Relationships on SO_2 Exposure

Abstract: We report a simple inorganic route for synthesizing a Pd/WO_3 3D hollow sphere nanocatalyst, where Pd nanoparticles are encapsulated and well distributed on porous tungsten oxide nanospheres. The synthesized nanocatalyst exhibited 100% CO to CO_2 conversion efficiency at 260 °C. In addition, the nanocatalyst demonstrated remarkable SO_2 (3 ppm) tolerance during the CO oxidation reaction for prolonged SO_2 sulfation of 1−21 h at 260− 400 °C. This represents the longest SO_2 exposure time reported to date based on a single metal Pd/support-based nanocatalyst. No decrement in CO conversion efficiency was observed even after SO_2 (3 ppm) treatment for 21 h for the first time based on a single metal Pd-based nanocatalyst.

Moreover, the synthesized nanocatalyst shows H_2S (4 ppm), even in situ H_2S tolerance during the CO oxidation reaction at 260 °C for 1−3 h and exhibited less sensitivity to prolonged and stringent sulfur exposure, with the highest H_2S concentration and maximum 100% CO to CO_2 conversion efficiency obtained after H_2S treatment for the first time based on a Pd-based nanocatalyst to the best of our knowledge. The composition and structure of the R-Pd/WO_3 nanocatalyst were not much influenced, even after the prolonged SO_2 and H_2S exposure during the CO oxidation reaction, as verified from spent catalyst analysis. Finally, our DFT-based model provides insights into understanding the observed sulfur resistance on Pd/WO_3 by analyzing the underlying electronic structure. Therefore, our strategic synthesis methodology will open up many opportunities to select Pd/metal oxide-based nanomaterials for designing highly efficient, stable, and SO_2/H_2S-resistant nanocomposite catalyst.

Keywords: palladium (Pd), tungsten oxide (WO_3), nanocatalyst, CO oxidation, SO_2 and H_2S resistant ability, DFT calculation.

Biography: In 2017, I've joined as a project assistant in CSIR-National Chemical Laboratory, Pune, India. After three years I've registered for the PhD program (Chemical Sciences) in Academy of Science and Innovative Research (AcSIR), India, under the guidance of Dr. Shatabdi Porel Mukherjee, Physical and Material Chemistry Division, CSIR- National Chemical Laboratory, Pune. I've successfully defended my PhD thesis titled "Synthesis of Oxide-based Nanomaterials: Catalysis, Electrocatlysis and Adsorption Applications" and rececived my PhD award on 23th November, 2024. During my research journey I've published five first author paper and one granted patent (In) and three complete filing patents (In and WO).