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Mechanistic Studies Of Co Oxidation Over Single Atom Catalysts Supported By Metal-organic Frameworks

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Metal-Organic Frameworks (MOFs) show great potential as ultrahigh surface area sorbents and catalysts for the capture of toxic compounds. In this work, the zirconium-based MOFs, UiO-66 and MOF-808, were synthesized with engineered missing linker defects, designed for post-synthetic coordination of single atoms of various transition metals. The ability of single atom metal-MOF based catalysts to oxidize small gas-phase compounds was discerned through a model reaction, the oxidation of CO. The reaction was performed in an ambient pressure packed-bed reactor coupled to an infrared spectrometer for identification of products. In determining the most optimal material for the conversion of CO to CO2, the identity of both the metal and support was varied. Preliminary findings suggest that MOF-808 outperforms UiO-66 as a support for the oxidation of CO, with enhanced reactivity when decorated with single atom platinum sites. Determining the most effective combination of the support and metal utilizing a model reaction allows for efficient screening of a wide range of materials, narrowing the focus to materials that show promise for oxidation of larger molecules, such as chemical warfare agents (CWAs). Incorporation of these materials into protective equipment would provide improved defense for the warfighter against exposure to harmful compounds that can be rendered non-toxic through oxidation.

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