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ABSTRACT:

A nanostructured hybrid catalyst for environmental applications: NO removal at rt.

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Air pollution is an epochal concern, and is linked to combustion processes, leading to the emission of nitrogen oxides (NOx), which constitutes a critical environmental problem, and it can affect severely human health. At ambient temperature and pressure, NOx decomposition is thermodynamically favoured; however, this process is kinetically inhibited, owing to a high activation energy. To date, no reported heterogenous catalyst possesses the required properties to lower the activation energy of this process without the help of co-reacting agents and high temperature. Nature resolves the denitrification problem with an assortment of different iron and copper based metalloenzymes, that sequentially reduce nitrate to dinitrogen via nitrogen oxide intermediates, e.g., nitrate reductase, nitrite reductase (NIR), nitric oxide reductase (NOR) and nitrous oxide reductase. Inspired by those structures, using DFT calculations, material design, advanced synthesis, and state-of-the-art characterisation methods we have been able to prepare a catalyst able to decompose NO at room temperature and in the presence of oxygen and water, without the assistance of a reducing species. The nano-structured material is an iron trimesate MIL-100(Fe), a bio-compatible Metal Organic Framework, easy to be scaled-up via green synthesis. Its reaction mechanism has been described using *operando* IR spectroscopy. This represents a leap forward in the comprehension of the deNOx mechanism, and allows to bridge the gap between heterogeneous and enzymatic catalysis, while using an inexpensive solution for air purification in specific confined polluted ambient.

[1] M. Daturi *et al*., Adv. Mater. 2024, 2403053.