
Single-atom Catalyzed Redox Reactions in the N₂O Couple: A Combined Experimental-Computational Approach

Helmut Schwarz

Institut für Chemie der Technischen Universität Berlin, 10623 Berlin.

Helmut.Schwarz@tu-berlin.de

Abstract

Arguably, the metal-mediated CO → CO₂ conversion constitutes one of the best-studied oxidation processes, both at surfaces and in the gas phase - and yet, many mechanistic details are shrouded in mystery.

In this lecture, in a combination of advanced mass spectrometry, gas-phase infrared spectroscopy and computational chemistry, the active site of heteronuclear metal oxides – the so-called "aristocratic atoms" – will be identified and detailed reaction pathways are suggested for the redox reaction N₂O + CO → N₂ + CO₂.

This unique approach also helps to provide a deeper understanding on the currently hotly debated subject of 'single-atom catalysis'.



