Helmut Schwarz et al., J Chromatogr Sep Tech 2015, 6:4
http://dx.doi.org/10.4172/2157-7064.S1.007

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International Summit on
Current Trends in Mass Spectrometry
July 13-15, 2015 New Orleans, USA

Ménage-à-trois: Single-atom catalysis, mass spectrometry and computational chemistry

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We shall present selected examples of gas-phase reactions which are of timely interest for the catalytic activation of small molecules. Due to the very nature of the experiments, detailed insight in the active site of catalysts is provided and – in combination with computational chemistry – mechanistic aspects of as well as the elementary steps involved in the making and breaking of chemical bonds are revealed. Examples to be discussed include inter alia: (i) Metal-mediated carbon-carbon bond formation; (ii) low-temperature, catalytic oxidation of CO; (iii) oxygen-centered radicals as active sites in catalytic hydrocarbon activation, e.g. the oxidative coupling of methane 2CH4→C2H6. It will be shown that mass-spectrometry based studies on 'isolated' reactive species provide an ideal arena for probing experimentally the energetics and kinetics of a chemical reaction in an unperturbed environment at a strictly molecular level, and thus enable the characterization of crucial intermediates that have previously not been within the reach of conventional condensed-phase techniques.

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