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Conversion of NO on Cerium Dioxide – Computational Modeling

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Extended Abstract

The main feature of cerium dioxide is the oxygen storage capacity, allowing release and accommodation of oxygen depending on the reaction conditions. The reduction of cerium dioxide results in formation of O vacancies, which is accompanied by reduction of two Ce^{4+} cations to Ce^{3+}. This behavior of cerium dioxide is found to depend strongly on the nanostructuring of the material [1,2]. In order to clarify the specific properties of nanosized particles of cerium dioxide we performed series of quantum chemical calculations of model systems containing pristine ceria nanoparticles, supported platinum species as active phase, doped structure with other metal ions, as well as intermediate surface species.

We investigated deposited platinum clusters and isolated ions on cerium dioxide support as well as adsorption and oxidation of CO or NO on them [3]. The relative stability of several reduced and oxidized structures as well as different locations of the platinum was modelled.

As surface intermediates for NO conversion we considered various structures of nitrites, nitrates, as well as some novel structures as new types of surface species as azides and nitric oxide dianion [4,5].

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