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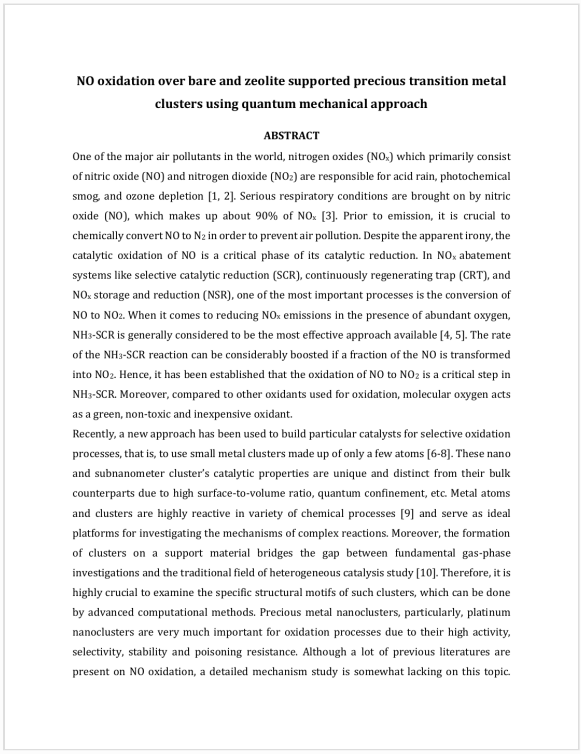

NO oxidation over bare and zeolite supported precious transition metal clusters using quantum mechanical approach

ABSTRACT

One of the major air pollutants in the world, nitrogen oxides (NO_x) which primarily consist of nitric oxide (NO) and nitrogen dioxide (NO_2) are responsible for acid rain, photochemical smog, and ozone depletion [1, 2]. Serious respiratory conditions are brought on by nitric oxide (NO), which makes up about 90% of NO_x [3]. Prior to emission, it is crucial to chemically convert NO to N_2 in order to prevent air pollution. Despite the apparent irony, the catalytic oxidation of NO is a critical phase of its catalytic reduction. In NO_x abatement systems like selective catalytic reduction (SCR), continuously regenerating trap (CRT), and NO_x storage and reduction (NSR), one of the most important processes is the conversion of NO to NO_2. When it comes to reducing NO_x emissions in the presence of abundant oxygen, NH_3-SCR is generally considered to be the most effective approach available [4, 5]. The rate of the NH_3-SCR reaction can be considerably boosted if a fraction of the NO is transformed into NO_2. Hence, it has been established that the oxidation of NO to NO_2 is a critical step in NH_3-SCR. Moreover, compared to other oxidants used for oxidation, molecular oxygen acts as a green, non-toxic and inexpensive oxidant.

Recently, a new approach has been used to build particular catalysts for selective oxidation processes, that is, to use small metal clusters made up of only a few atoms [6-8]. These nano and subnanometer cluster's catalytic properties are unique and distinct from their bulk counterparts due to high surface-to-volume ratio, quantum confinement, etc. Metal atoms and clusters are highly reactive in variety of chemical processes [9] and serve as ideal platforms for investigating the mechanisms of complex reactions. Moreover, the formation of clusters on a support material bridges the gap between fundamental gas-phase investigations and the traditional field of heterogeneous catalysis study [10]. Therefore, it is highly crucial to examine the specific structural motifs of such clusters, which can be done by advanced computational methods. Precious metal nanoclusters, particularly, platinum nanoclusters are very much important for oxidation processes due to their high activity, selectivity, stability and poisoning resistance. Although a lot of previous literatures are present on NO oxidation, a detailed mechanism study is somewhat lacking on this topic.

NO oxidation over bare and zeolite supported precious transition metal clusters using quantum mechanical approach

by Nishant Biswakarma

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