# 2002 Quantum chemical molecular dynamic simulation of NO adsorption on supported Pt catalyst

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## 1. Introduction

Reduction of NO on the γ-$Al_2O_3$ supported Pt metal surface is one of the major reactions in three-way catalytic converter. Adsorption of NO on Pt surface is the elementary step for further dissociation reaction. In this study, we investigated the dynamics of adsorption of NO on γ-$Al_2O_3$ supported $Pt_4$ metal cluster surface by using our original tight-binding quantum chemical molecular dynamics simulator, New-Colors.

## 2. Method

'New-Colors' program is based on our tight-binding quantum chemical molecular dynamics program, Colors [1]. In New-Colors program, total energy of a system is evaluated by the following equation:

$$E = \sum_{i=1}^{N} \frac{1}{2} m_i v_i^2 + \sum_{k=1}^{occ} n_k \varepsilon_k + \sum_{i=1}^{N} \sum_{j=i+1}^{N} \frac{Z_i Z_j e^2}{r_{ij}} + \sum_{i=1}^{N} \sum_{j=i+1}^{N} E_{ij}^{repul}(r_{ij}) + \sum_{i=1}^{N} E_{corr}(Z_i)$$

where the first, second, third, fourth, and fifth term in the above equation refers to the kinetic energy of nuclei, band energy, Coulombic energy, exchange-repulsion energy, and correction energy, respectively.

## 3. Results and Discussion

We optimized the structure of the NO/$Pt_4$/γ-$Al_2O_3$ (NO at atop) by using the periodic DFT calculation program, DMol[3], as the initial for dynamic simulation [1]. Quantum chemical molecular dynamics simulation was carried out for 5000 steps with the integration time of $0.1 \times 10^{-15}$ s. Temperature of the system is set to 900 K. Figure 1 shows that the NO molecule changes from atop linear to atop bent position at 4400 steps. Thus the vibration modes of the NO bond changes. It is very clear from the N-O bond length vs calculations step plot in Figure 2, where the pattern of the plot changes after 4400 step. Experimental investigation also reported the existence of bent Pt-NO species [2]. The possible explanation of this behavior is the change in bond order of NO, i.e., the bent position of NO do not permits it to accept the electron density in $2\pi^*$ orbital from Pt atom effectively as that for linear position.

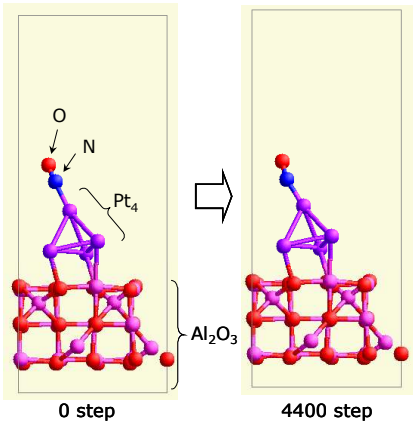


Fig. 1 Dynamics of NO adsorption on $Pt_4$/γ-$Al_2O_3$ surface.

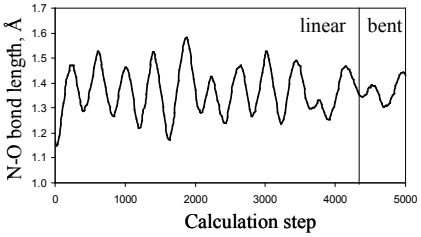


Fig. 2 Change of NO bond length with calculation step

**References:**

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