

Dissociation of nitrous oxide on a Pd(110) surface

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Nitrous oxide, N₂O, has attracted increasing attention as a greenhouse gas and also as an intermediate in the removal of NO_x on automobile three-way catalysts. However, the mechanism of its decomposition and formation on the catalysts is not yet clear. The unusual inclined N₂ desorption observed recently during thermal dissociation of N₂O over Pd(110), Rh(110) and Ir(110) is expected to provide more insight into the dynamics of its emission. Two different explanations of this inclined desorption of N₂ have been given. Haq *et al.* [1] suggested the inclination to be due to the reconstructed surface from which N₂ desorbs along the local surface normal. An alternative mechanism, which also works well with the non-reconstructed surface, was provided by Matsushima [2].

In this contribution, results of DFT-GGA calculations applied to the characterization of the adsorption and dissociation of N₂O on Pd(110) surface are presented. Two stable adsorption forms were found [3], where N₂O adsorbs either in a tilted form with the terminal N atom attached to the surface, or horizontally on the surface in the [001] direction. In the latter form, which can explain the inclined desorption, adsorbed N₂O is bent with its O atom pointing to the surface. The activation barrier for dissociation was found to be a strong function of the adsorbate coverage.

[1] S. Haq, A. Hodgson, *Surf. Sci.* **463**, 1 (2000).

[2] T. Matsushima, *Catal. Surveys from Japan* **5**, 71 (2002).

[3] A. Kokalj, I. Kopal, H. Horino, Y. Ohno, T. Matsushima, *Surf. Sci.* **506**, 196 (2002).

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