第150回触媒化学研究センター談話会

演　題：A DFT Computational Study of the Structures of N_2O Adsorbed on Pd and Rh Surfaces

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14:00－15:30

会　場：北海道大学理学部本館S302

要　旨：The structure of adsorbed nitrous oxide, N_2O, is an important ingredient for understanding the mechanism of the peculiar inclined N_2 desorption observed during thermal dissociation of N_2O on Pd(110),Rh(110) and Ir(110) [1]. We have studied and characterised the adsorption of N_2O on Pd and Rh surfaces using density-functional theory. We found that N_2O binds to the (110) surfaces in two alternative forms, either tilted with the terminal N atom attached to the surface, or lying horizontally on the surface in the [001] direction. The tilted form remains linear on adsorption, while the horizontal form is bent, with the terminal-nitrogen and oxygen atoms pointing towards the surface. N_2O binds more strongly to the Rh(110) surface--a consequence of the less occupied d-bands of the rhodium substrate. The Pd(100) surface behaves differently. On this surface, the tilted $N_2O(a)$ form is substantially preferred, and the binding of the horizontal form to the surface is questionable due to very small adsorption energies, E_{ads}<0.1 eV. The calculations suggest that the structures of adsorbed N_2O are surface structure sensitive. In particular, the structure of a surface appears to be more important factor than the kind of the substrate metal in determining the structures of $N_2O(a)$. The effect of adsorbed oxygen on the adsorption energetics and structures of $N_2O(a)$ will be also briefly discussed.

[1] H. Horino, I. Rzeznicka, A. Kokalj, I. Kobal, Y. Ohno, A. Hiratsuka, T. Matsushima, J. Vac. Sci. Tecnol. A 20, 1592 (2002)

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