MS18-P07 | FIRST-PRINCIPLES STUDY OF OXYGEN ADSORPTION STRUCTURE ON Ni_3Al(210) SURFACE

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Recently, it was reported that Ni_3Al is highly active for hydrogen production from methanol and methane, and its catalytic performance is considered to be attributed to the selective oxidation and hydroxylation of Al and the formation of metallic Ni particles at low oxygen partial pressures [1,2]. In order to reveal the details of the initial oxidation process, we are studying the stable adsorption structure of oxygen on the Ni_3Al (210) surface using the first-principles calculation based on the density functional theory. For low coverage surfaces (0.25 and 0.5 ML), the most stable adsorption site is a pseudo-threefold hollow site surrounded by two Al atoms and Ni atom, implying partial oxidation of surface Ni. Although the atomic arrangement of surface atoms and the adsorbed oxygen atom of the most stable adsorption structure is very similar to the reported most stable adsorption structure on the NiAl (110) surface [3], the oxidation behavior of the surface Ni atom may disagree with the recent experiment, which did not observe the sign of the Ni oxidation at the initial stage of the oxidation process [4]. We will also discuss the electronic structure of the surface atoms and stable adsorption structures taking into account the exchange of atoms between different atomic layers.

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