MS18-P04 | AB-INITIO STUDY OF OXYGEN ADSORPTION ON PDZN(111) SURFACE

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Pd is highly active for the decomposition of methanol, but it becomes active for methanol steam reforming when alloying with Zn [1, 2]. A close connection between the catalytic property and the d-band structure was pointed out, and it is confirmed that PdCd, showing very similar d-band structure with PdZn, exhibits comparable catalytic property with PdZn [2, 3]. The change in the d-band structure, namely, leads to the change in the catalytic property. This change in the d-band structure was also clearly demonstrated by electronic structure calculations based on the density functional theory (DFT) [4]. However, a different origin of the change in the catalytic property was proposed for the isostructural intermetallic compound NiZn, and it was concluded that the desegregation of the NiZn surface by Zn oxidation is essential [5]. Needless to say, understanding the mechanism of the change in the catalytic property is important, thus, we are carrying out plane-wave DFT calculations to investigate the effect of oxidation on the electronic structure of PdZn. In this presentation, we will discuss the optimal structure of oxygen-adsorbed PdZn(111). surface.

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