Electronic structure and magnetism of catalytic material Pt_3Ni surfaces: Density-functional study

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Abstract

A Pt-skin $Pt_3Ni(111)$ surface was reported to show high catalytic activity. In this study, we investigated the magnetic properties and electronic structures of the various oriented surfaces of bulk-terminated and Pt-segregated Pt3Ni by using a first-principles calculation method. The magnetic moments of Pt and Ni are appreciably enhanced at the bulk-terminated surfaces compared to the corresponding bulk values, whereas the magnetic moment of Pt on the Pt–segregated $Pt_3Ni(111)$ surface is just slightly enhanced because of the reduced number of Ni neighboring atoms. Spin-decomposed density of states shows that the dz2 orbital plays a dominant role in determining the magnetic moments of Pt atoms in the different orientations. The lowering of the d-band center energy (-2.22 eV to -2.46 eV to -2.51 eV to -2.65 eV) in the sequence of bulk-terminated (100), (110), (111), and Pt-segregated (111) may explain the observed dependence of catalytic activity on surface orientation. Our d-band center calculation suggests that an observed enhanced catalytic activity of a $Pt_3Ni(111)$ surface originates from the Pt-segregation.

Keywords: Pt_3Ni, density-functional theory, magnetism, electronic structure, catalytic activity