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Theoretical investigation of CO oxidation on AuAg (110) alloy surface. JYH PIN CHOU, IAMS, Academia Sinica, Taipei, Taiwan and National Chung Cheng University, Chia-Yi, Taiwan, CHING-MING WEI, IAMS, Academia Sinica, Taipei, Taiwan — Carbon monoxide (CO) oxidation on the gold-silver (110) binary alloy surface has been investigated by using density functional theory. For clean metal (110) surface, it was found that CO prefers to adsorb on atop and short bridge site of Au(110) surface [1] and O_2 prefers to adsorb on fourfold hollow (FFH) site of Ag(110) surface [2]. In this work, we present the results of CO, O_2 adsorption, and CO+O_2 coadsorption on AuAg(110) surface. The results indicate that the adsorption energies are mainly determined by the type of atoms on the bonding site. For CO, adsorption on Au atop and Au_2 short bridge site are favored and have an adsorption energy range of 0.43∼0.63 eV. For O_2, adsorption on FFH site with $Au_{5-n}Ag_n$ (n≧3) configuration is possible and has an adsorption energy range of 0.12∼0.53 eV. For CO+O_2 coadsorption, the coadsorption energy on $Au_{5-n}Ag_n$ (n≧3) FFH site is slightly less than the sum of CO and O_2 adsorption energy by only 0.05∼0.1 eV. The oxidation of adsorbed CO with O_2 is found to proceed via formation of an intermediate, OCOO, and has a surprising low energy barrier of 0.2∼0.3 eV. [1] Tatyana E. Shubina, Christoph Hartnig and Marc T. M. Koper, Phys. Chem. Chem. Phys. 6, 4215,(2004) [2] P. A. Gravil and D. M. Bird, Phys. Rev. Lett. 77, 3993(1996)

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