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NCO and OCN adsorption and decomposition study on the Ag(110) surface

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The adsorption of C, N, O, CO, CN, NCO and OCN, as well as CO, CN, NCO and OCN decomposition on Ag(110) surface were studied by using the density functional theory (DFT) combined with the periodic slab model. Preferential site of each adsorbate has been determinated : C, N and O (hollow site), CO and CN (top site), NCO (long bridge site) and OCN (short bridge site). Work function and dipole moment changes allowed us to determine the direction of charge transfer. We evaluated diffusion barrier of all adsorbates and analyzed the interaction between the adsorbate and the surface, in the framework of the local density of states. Thermochemical decomposition of CO,CN, NCO and OCN on Ag(110) surface has been found energetically unfavorable. The CI-NEB calculations of decomposition of CO, CN, NCO and OCN on Ag(110) also shown that, the decomposition reactions CO, CN, NCO and OCN on Ag(110) are endothermics.

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