

Using spin polarized DFT, we performed mechanistic studies of methane dry reforming on Cu-Ni bimetallic surfaces. We computed the local density of states (LDOS) of intermediates/surfaces to analyse chemical bonding on different Cu-Ni alloys. Our results show that carbon resistance of low Cu amount surfaces is related to a reduced interaction of CH 1π orbital with 3d states. Likewise, the lowering of (1π , $2\pi^*$ - 3d) binding intensity, catalyses CO desorption rather than its retention and/or activation, enhancing CO anti-poisoning.