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Chemical Bonding and Surface Electronic Structures of Pt3Co (111), Pt3Ni (111) Single Crystals

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With angle resolved photoemission spectroscopy (ARPES), the surface electronic band structures of Pt3Co (111) and Pt3Ni (111) single crystals are investigated, which allow to study the bonding interaction between chemically absorbed atomic oxygen and its surfaces. The d-band electrons of subsurface TM are separated from the direct chemical bonding with atomic oxygen. That is, the TM does not contribute to direct chemical bonding with oxygen. From the density functional theory (DFT) calculations, it is identified that the main origin of improved oxygen absorption property, i.e. softening of Pt-O bonding, is due to the suppression of Pt surface-states which is generated from change of interlayer potential, i.e. charge polarization, between Pt-top and TM-subsurface. Our results point out the critical roles of subsurface TM in modifying surface electronic structures, which in turn can be utilized to tune surface chemical properties.

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