Investigation of Thin Cobalt/Nickel/Manganese Oxides Supported on Au(111) and Other Fcc Metals

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In the last decade, a number of experiments have shown that ultra-thin layers of TMOs can be stabilized when interfaced with precious metal supports such as Au(111) and Pt(111) or Ir(100).[1–6] Moreover, gold supported Co/Ni/Mn-based catalysts have been experimentally proven to exhibit higher oxygen evolution reaction (OER) activities than other metal supported oxide catalysts.[7–9] However, the synergistic effect of contact with gold support is yet to be fully understood.

In the first half of my talk, I will report the results of our combined experimental and computational study of ultra-thin layered cobalt oxides.[4] The synthesis of three distinct types of thin-layered cobalt oxide nano-islands supported on a single crystal gold (111) substrate is confirmed by combination of STM, XAS methods. Additionally, DFT+U theoretical investigation of above nano-islands confirms stability of two low-oxygen pressure phases: (a) rock-salt Co-O bilayer and (b) wurtzite Co-O quadlayer and single high-oxygen pressure phase: (c) O-Co-O trilayer. Very importantly, I will discuss the effect of water exposure in these systems, which results in noticeable hydroxylation of the basal planes. The results of the theoretical hydroxylation models will be compared with experiments.

In the second half of my talk, I will present the calculated OER activities of general thin-film Mn/Fe/Co/Ni supported oxides, which are assumed to have the structure of the ultra-thin layered cobalt oxides. In more detail, I will discuss the theoretical overpotentials obtained on basal planes relative to edge sites in these systems as function of different metal support with the goal of elucidating the synergistic effect of gold.

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