Electronic structure of CoO nanoislands on Au(111)

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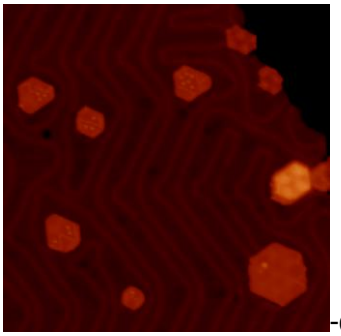
Oxides have found applications in various problems in the fields of chemistry, physics and materials science, notably for use in catalysis, encouraging investigation of fundamental properties of oxides. Hereby, transition metal oxides have been proposed as promising catalysts in the oxygen evolution reaction for water spliting, of crucial relevance in clean energy. Equipped with state-of-the-art scanning probe and sample-average techniques atomistic insights for FeO [1] and CoO [2], [3] and their activity towards water splitting have been recently reported.

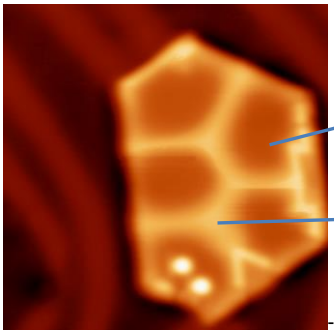
Despite this activity, there is a lack of knowledge about the precise electronic structure of most of these oxides. To understand better the activity of such catalysts, we have selected CoO nanoislands as an archetype model catalyst for water splitting. Our results show the emergence of a Moiré geometric and electronic pattern within the CoO nanoislands, revealing higher density of states in the conduction band at the top moirons inside the nanoislands, while showing an increase of the valence band states at the borders of the islands and at the bottom moirons inside the nanoislands.

The exposure of such catalyst to water highlights that catalyst activity towards water splitting depends on substrate temperature. At room temperature [3], the water is adsorbed and dissociated, affording the formation of hydroxyls, which are located predominantly at the bottom moirons. However, at low temperatures the water is adsorbed intact exclusively on the bottom moirons and can be manipulated with the STM tip, affording a multi-level electronic molecular nano-switch.

Our results shed light into the atomistic adsorption and dissociation of water on a very promising catalysts and reveal that such a process is temperature dependent.



-0.3 V, 61nmx61 nm



-0.3V, 15.1nmx15.1nm

References:

[1]: Parkinson, G. S., Novotný, Z., Jacobson, P., Schmid, M. and Diebold, U. J. Am. Chem. Soc., **133** (32), 12650-12655 (2011).

[2]: Fester, J., García-Melchor, M., Walton, A. S., Bajdich, M., Li, Z., Lammich, L. and Lauritsen, J. V. Nat commun, **8**, 14169 (2017).

[3]: Walton, A. S., Fester, J., Bajdich, M., Arman, M. A., Osiecki, J., Knudsen, J. and Lauritsen, J. V. Acs Nano, **9** (3), 2445-2453 (2015).