

What is the real state of single-atom catalysts under electrochemical conditions – from adsorption to surface Pourbaix Plots?

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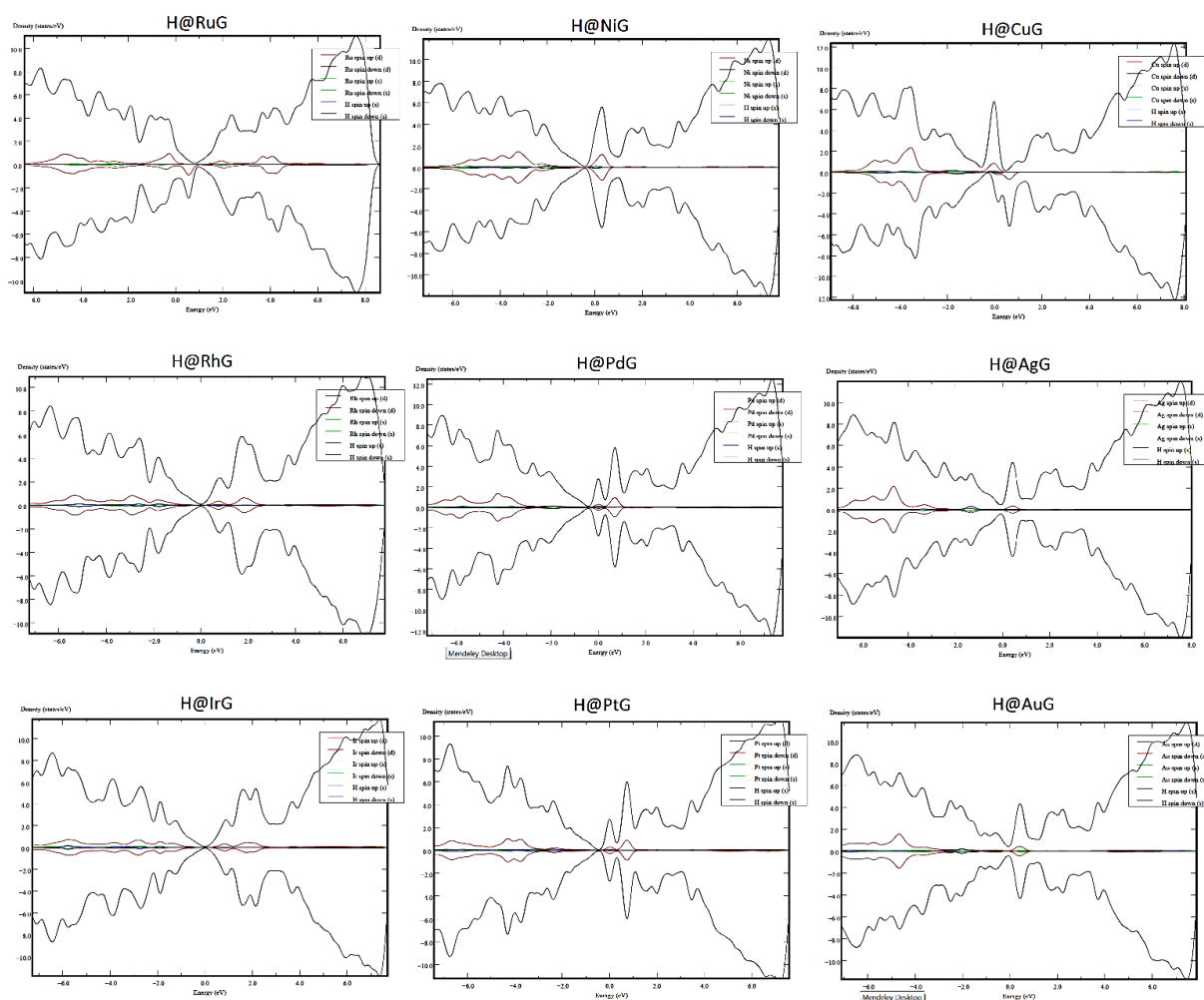


Figure S1. Densities of states for the investigated M@vG systems with adsorbed hydrogen. Total DOS, metal d- and s-states and H s-states are given.

SUPPLEMENTARY INFORMATION

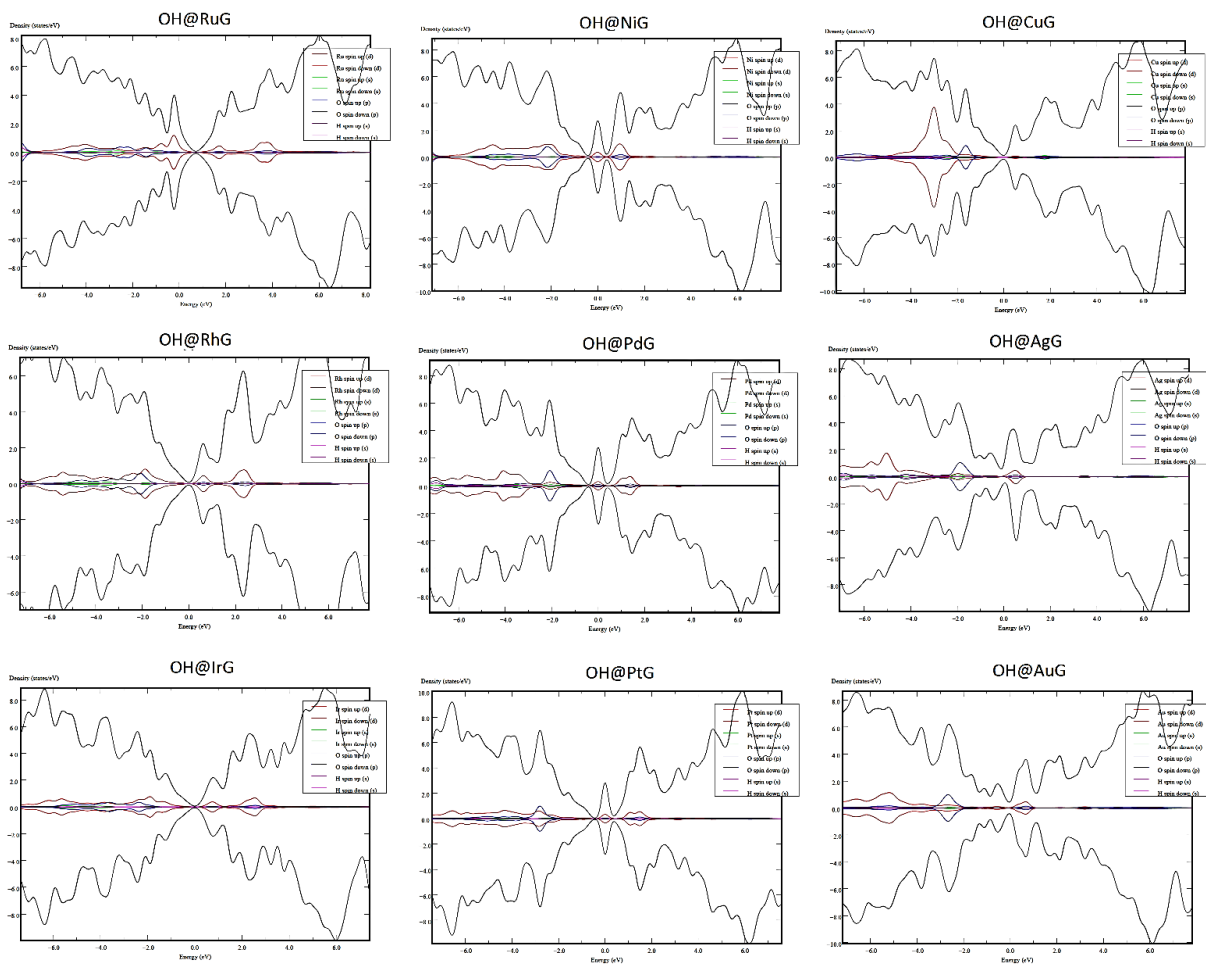


Figure S2. Densities of states for the investigated M@vG systems with adsorbed OH. Total DOS, metal d- and s-states, O p- and H s-states are given.

SUPPLEMENTARY INFORMATION

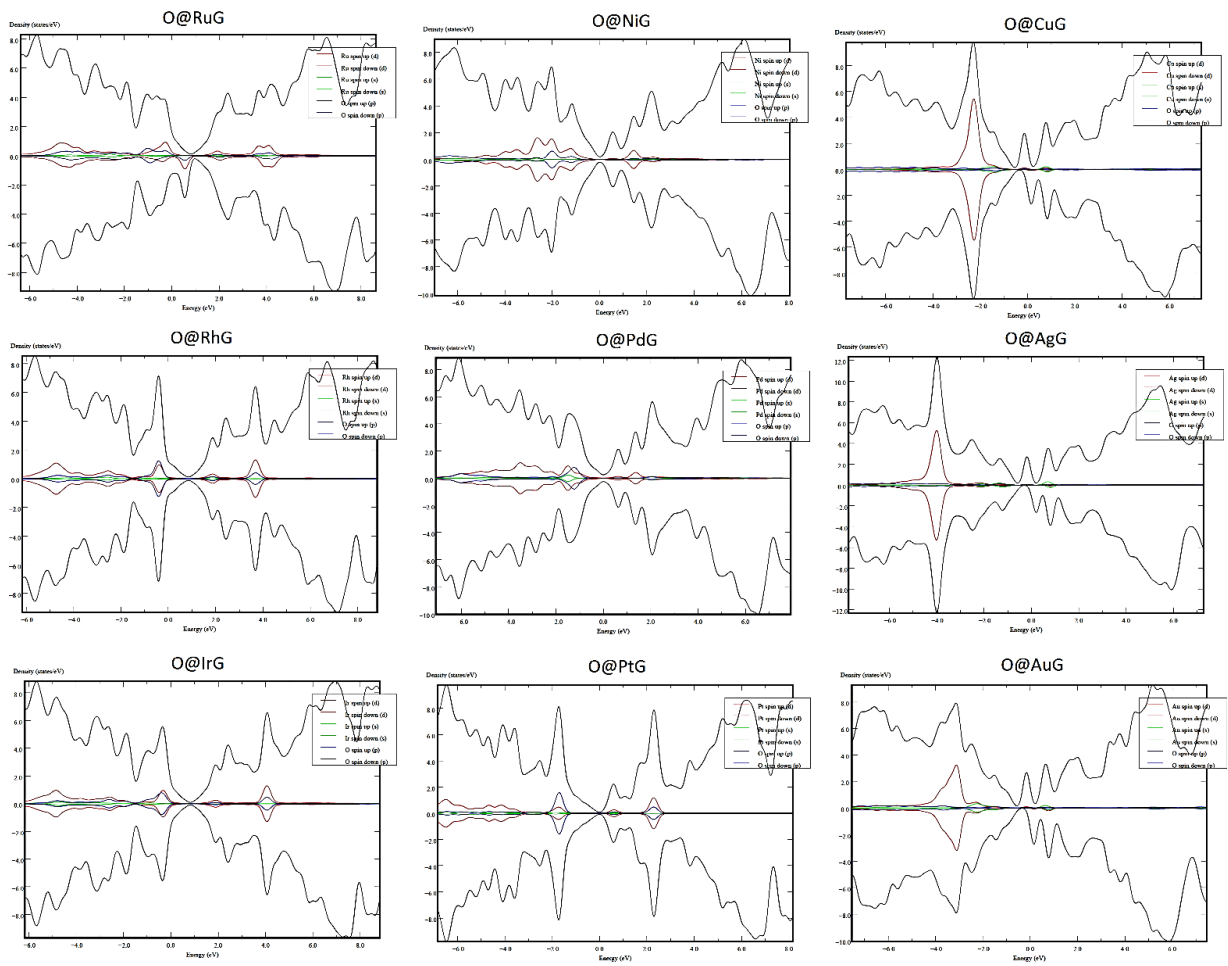


Figure S3. Densities of states for the investigated M@vG systems with adsorbed O. Total DOS, metal d- and s-states and O p-states are given.