Supporting Information

for

The role of oxygen and water on molybdenum nanoclusters for electro catalytic ammonia production

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Additional Figures

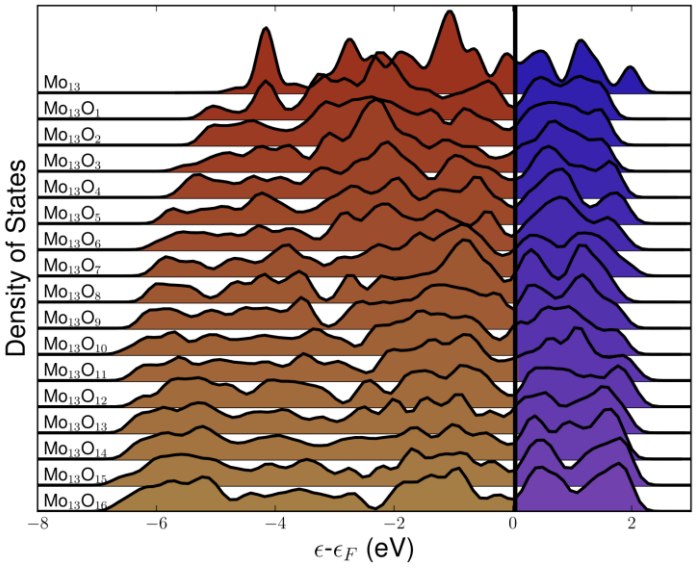

Figure S1: The d-band of molybdenum nanoclusters as the oxygen coverage evolves.

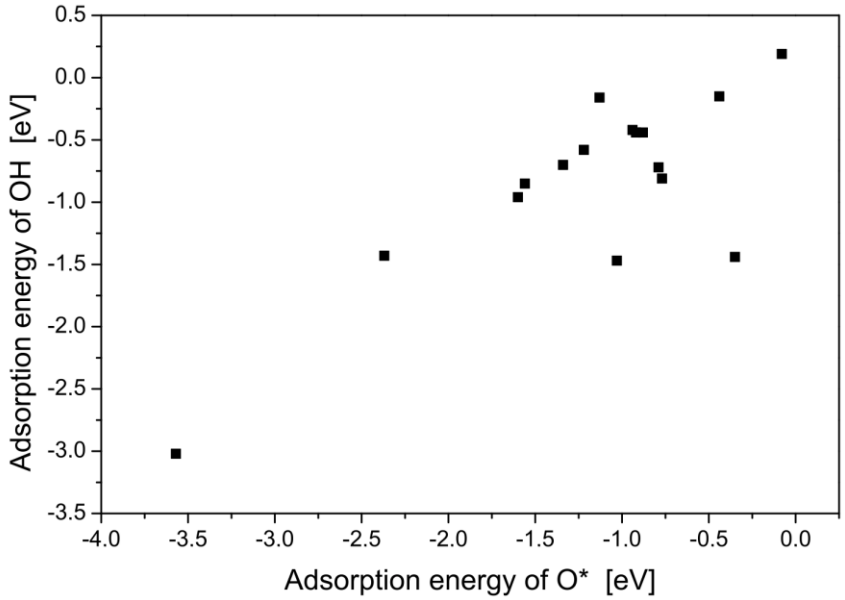

Figure S2: The adsorption energy of OH plotted as a function of adsorption energy of O for the oxygen covered molybdenum nanoclusters.

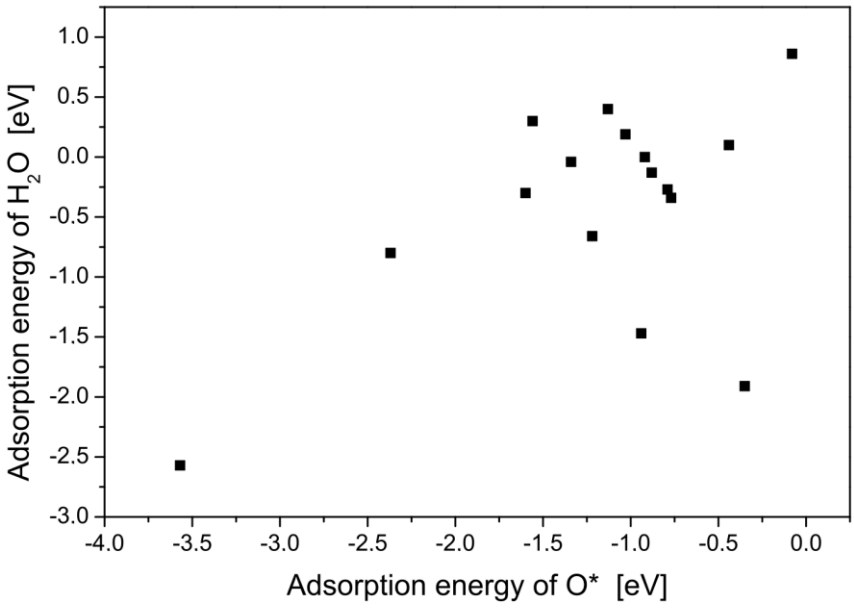

Figure S3: The adsorption energy of H_2O plotted as a function of adsorption energy of O for the oxygen covered molybdenum nanoclusters.