INSIGHTS ON HYDROGEN LIBERATION FROM WATER USING ANIONIC TRANSITION METAL OXIDE CLUSTERS: A COMBINED COMPUTATIONAL AND SPECTROSCOPIC STUDY

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Transition Metal Oxides (TMOs) offer widespread applications in catalysis and the generation of alternate sources of energy. Cluster models are useful to model the defect sites in these TMO surfaces which are responsible for their catalytic activities. In this combined computational (DFT) and spectroscopic (PES/MS) study, we present the interesting features in the chemical reactions of molybdenum oxide and tungsten oxide clusters with water. The results obtained provide valuable insights on the roles played by differing metal-oxygen bond strengths, the initial electrostatic complex formed and the geometric factors involved in the liberation of hydrogen gas from water.