ELUCIDATION OF PROTON-ASSISTED FLUXIONALITY IN TRANSITION-METAL OXIDE CLUSTERS

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The phenomenon of fluxionality in the reactions of transition-metal oxide clusters provides many opportunities in various industrial and catalytic processes. We present an electronic structure investigation of the fluxionality pathways when anionic W3O6 and Mo3O6 clusters react with three small molecules - water, ammonia and hydrogen sulfide. The presentation features a detailed understanding of (a) how the fluxionality pathway occurs and (b) the various factors that affect the fluxionality pathway - such as the metal, different spin-states and the nature of the non-metal in the reacting small molecule.