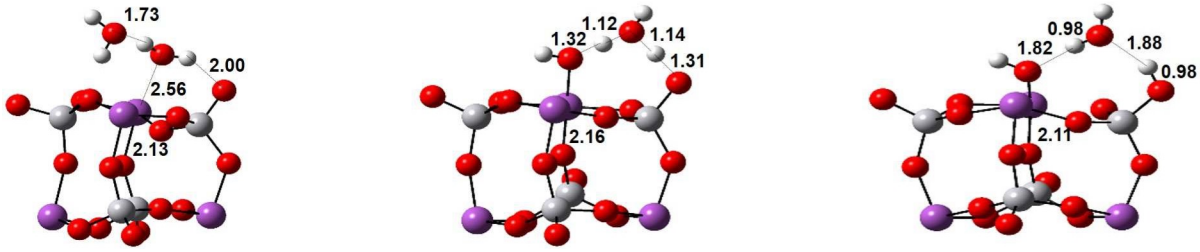
Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Electronic Supplementary Information
Water oxidation catalysed by quantum-sized $BiVO_4$

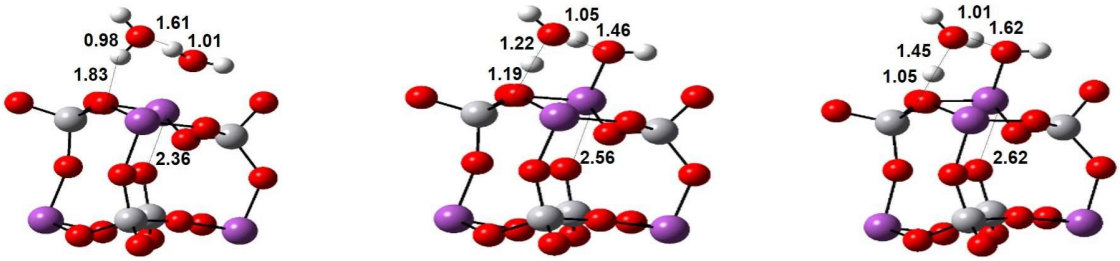
Optimised structures

Neutral pathway A



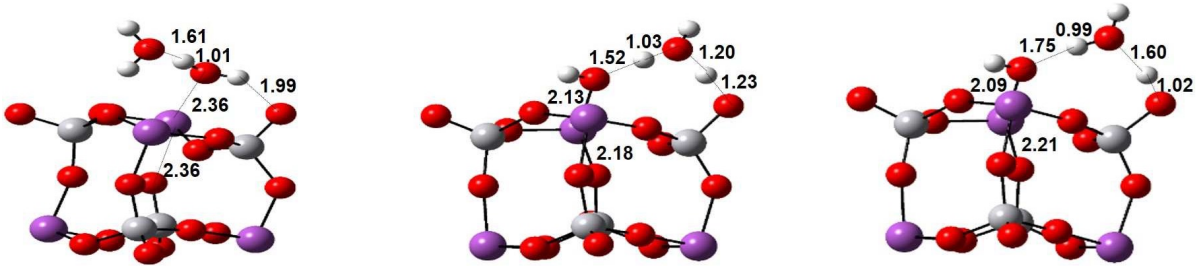
Reactant **Transition State** **Product**

Cationic pathway A



Reactant **Transition State** **Product**

Cationic pathway B

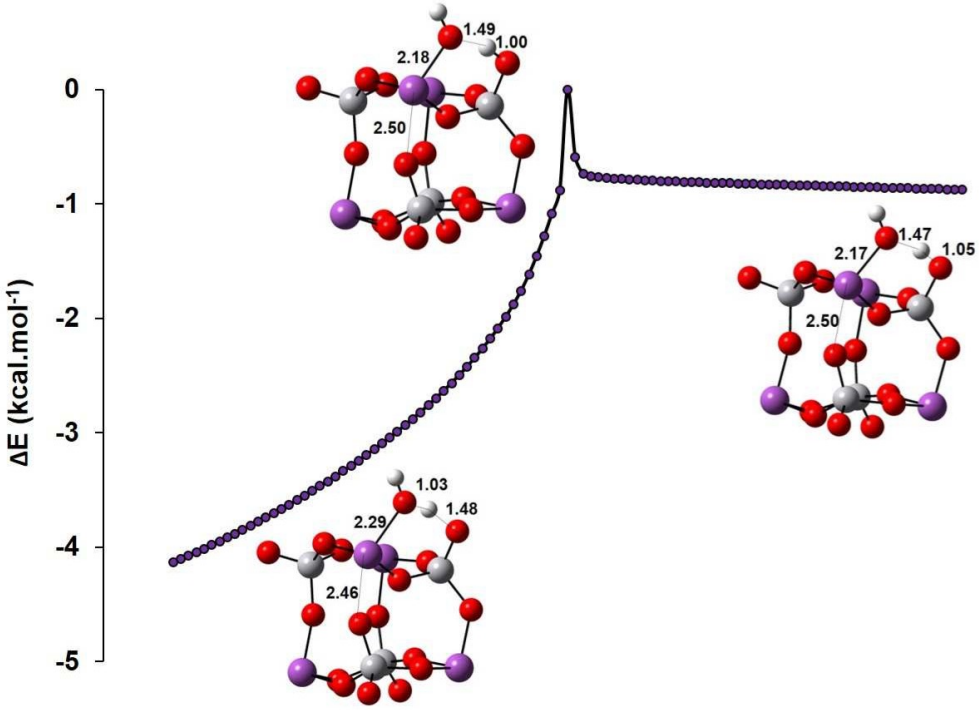


Reactant **Transition State** **Product**

Figure S1: Structures of the reactant, transition state and product for pathways A and B in the neutral and cationic regimes, calculated at B3LYP-D3/def-TZVP level of theory.

Intrinsic Reaction Coordinates

Pathway A



Pathway B

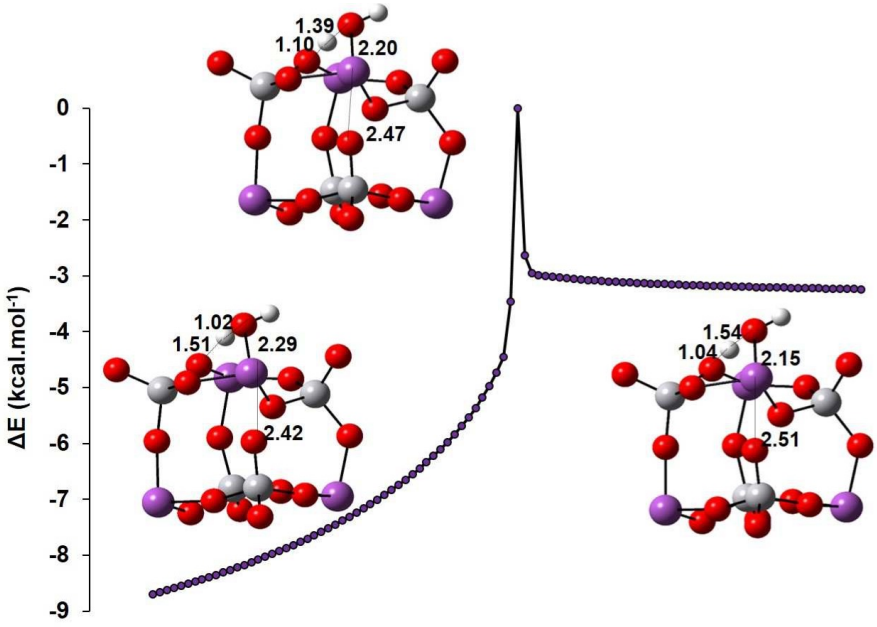


Figure S2: Intrinsic reaction coordinates for pathways A and B , calculated at B3LYP-D3/def-TZVP level of theory.

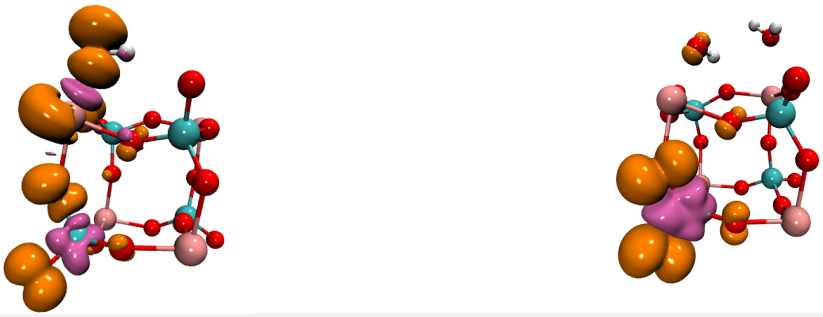


Figure S3: Spin densities of the $[(BiVO_4)_4\text{-}OH]^-$ and $[(BiVO_4)_4\text{-}OH(H_2O)]^-$ clusters