Supplementary Material (ESI) for PCCP

Interpretation of the $\tilde{A} \leftarrow \tilde{X}$ transition of hydrated proton in aqueous solution observed in far-UV region with quantum chemical calculations

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Figure S1

Ground (bottom) and excited state (top) NTOs of the first (left) and second shell (right) of $H^+(H_2O)_6$ optimized with the DFT (M062X/6-311++G(d,p)) method.