

## Electronic Supporting Information

Fig. S1 Molecular orbitals of  $\text{UO}_2\text{Cl}^+(\text{aq})$

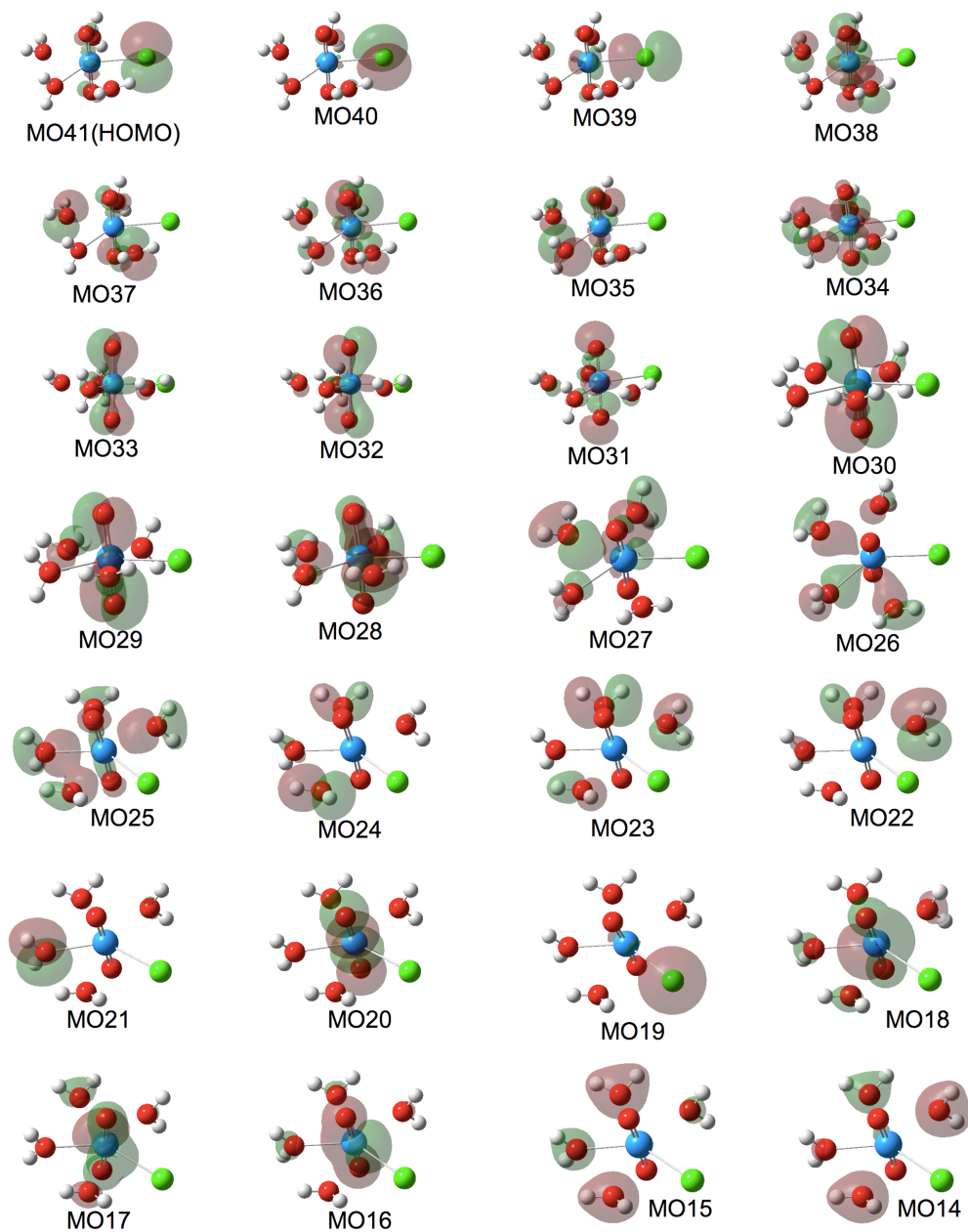


Fig. S2 Molecular orbitals of  $\text{UO}_2\text{F}^+(\text{aq})$

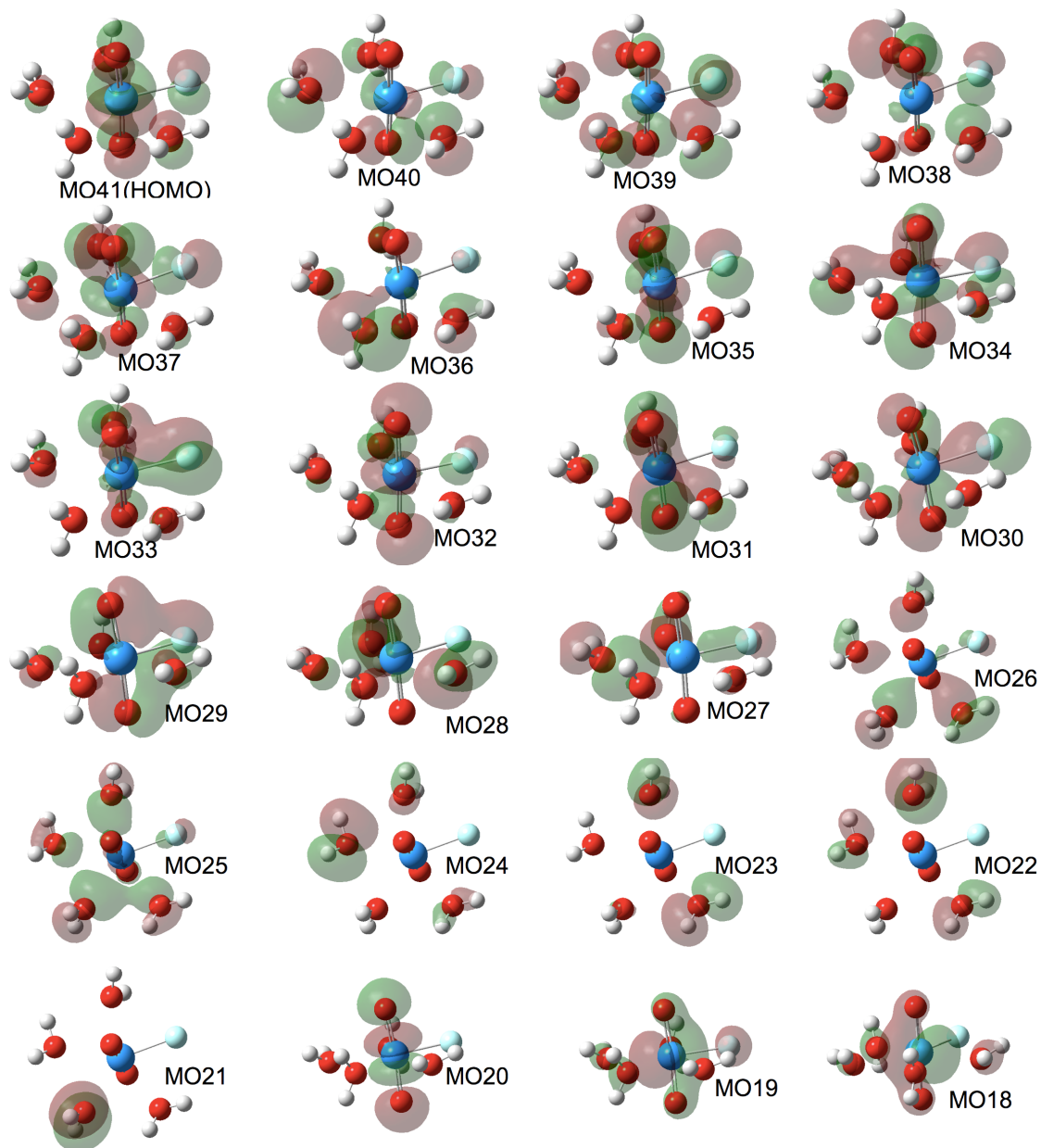


Fig.S3 Molecular orbitals of  $\text{UO}_2\text{OH}^+(\text{aq})$

