Supporting Information for

Ab initio electronic structure study of a model water splitting dimer complex

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Figure S1. Occupied UHF/TZVP alpha orbitals 50-62 in the nonet state of structure 1 (Contour value = 0.05).
Figure S2. UHF/TZVP alpha orbitals 87-96 in the nonet state of structure 1 (Contour value = 0.05). Orbitals 87-94 are occupied and 95-96 are unoccupied.

Figure S3. Occupied UHF/TZVP beta orbitals 79-86 in the nonet state of structure 1 (Contour value = 0.05)
Figure S4. Unoccupied UHF/TZVP beta orbitals 87-96 in the nonet state of structure 1 (Contour value = 0.05)
**Figure S5.** CASSCF(7,10)/TZVP active space natural orbitals in the octet state of structure 2

**Figure S6.** CASSCF(7,10)/TZVP natural core orbital 69 in the octet state of structure 2 (Contour value = 0.05)