Supplementray Information to:

Water activation by small free ruthenium oxide clusters

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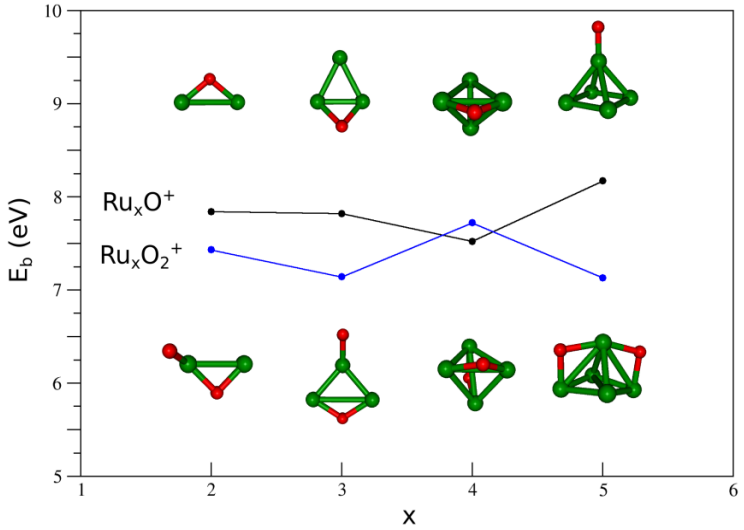

Fig. S1 Calculated O-atom binding energies for ruthenium mono- and di-oxides together with the corresponding lowest energy structures. E_b = E[Ru_xO^+] - E[Ru_x^+] - E[O] and E_b = E[$Ru_xO_2^+$] - E[Ru_xO^+] - E[O]. Ru and O atoms are indicated by green and red spheres, respectively.

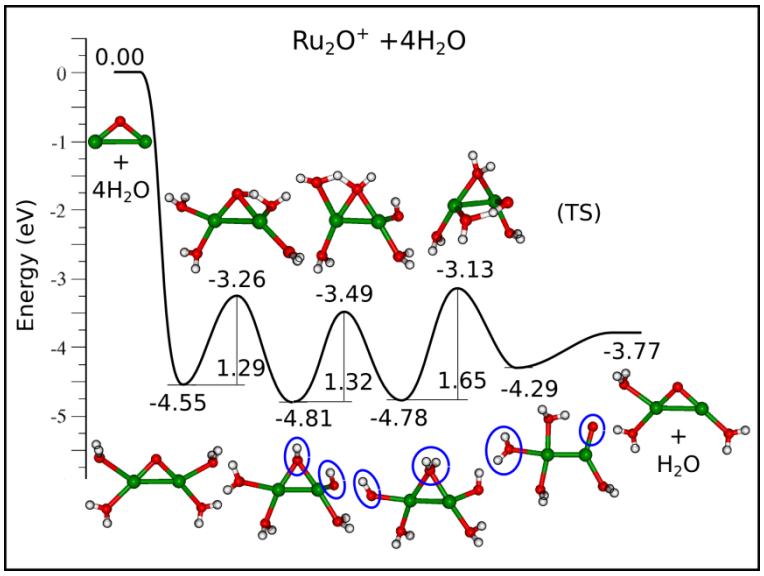

Fig. S2 Calculated energy profile of one possible reaction pathway for the [1,3] shift hydrogen transfer reaction of Ru_2O^+ + 4 H_2O including the lowest energy isomer depicted in Fig. 4b. Ru, O, and H atoms are indicated by green, red, and white spheres, respectively. The blue circles indicate the OH-groups resulting from the stepwise hydrogen shifts.

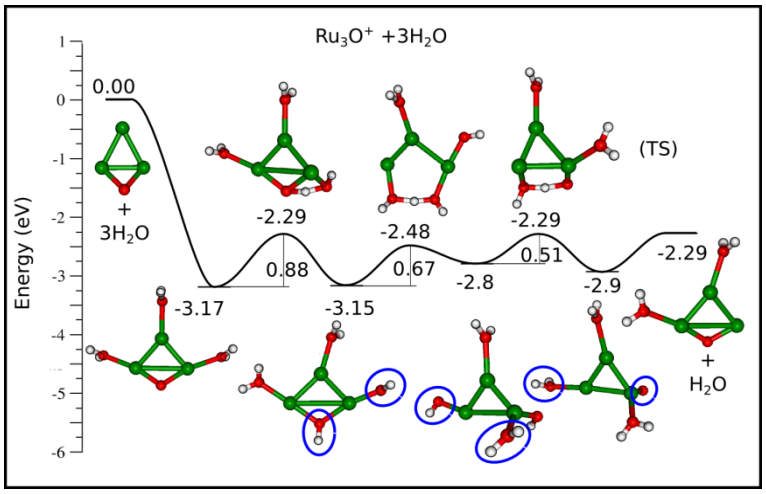

Fig. S3 Calculated energy profile of one possible reaction pathway for the [1,3] shift hydrogen transfer reaction of $Ru_3O^+ + 3\ H_2O$ including the lowest energy isomer depicted in Fig. 4d. Ru, O, and H atoms are indicated by green, red, and white spheres, respectively. The blue circles indicate the OH-groups resulting from the stepwise hydrogen shifts.

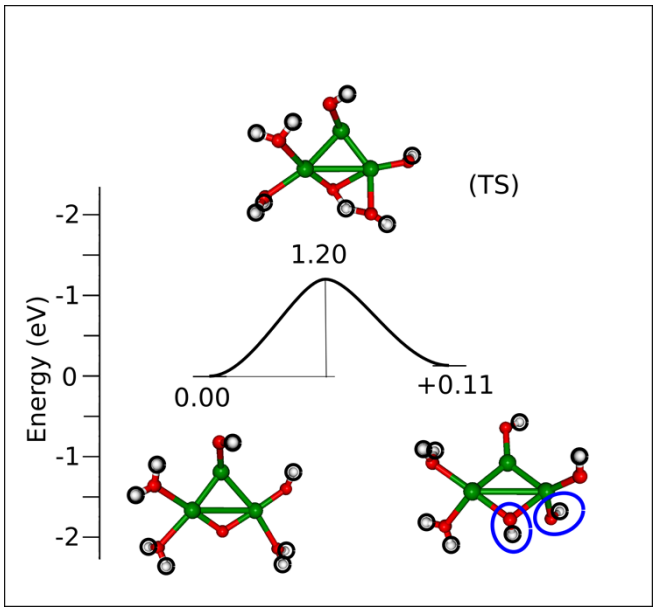

Fig. S4 Calculated energy profile for one possible reaction pathway for the [1,3] shift hydrogen transfer reaction of $Ru_3O(OH)_2(H_2O)_3^+$ yielding $Ru_3(OH)_4(H_2O)_2^+$. The initial structure $Ru_3O(OH)_2(H_2O)_3^+$ corresponds to the lowest energy isomer depicted in Figs. 4e and 6a. The blue circles indicate the OH-groups resulting from the hydrogen shift.

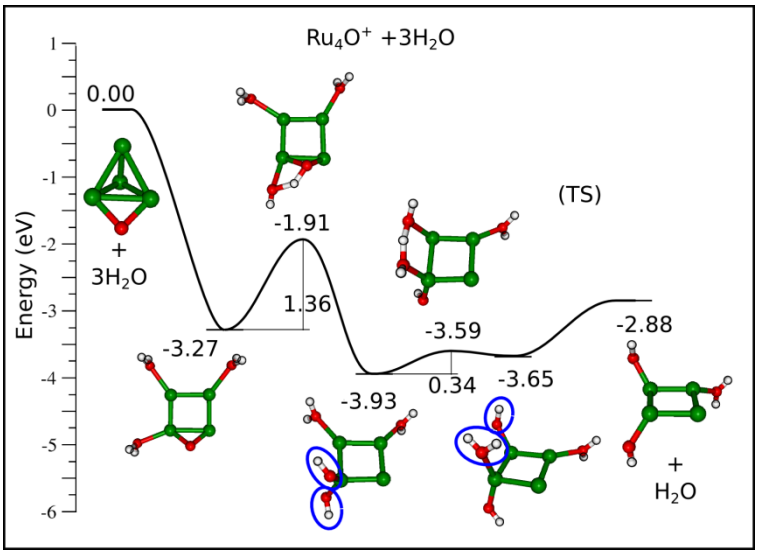

Fig. S5 Calculated energy profile of one possible reaction pathway for the [1,3]-shift hydrogen transfer reaction of $Ru_4O^+ + 3\ H_2O$ including the lowest energy isomer depicted in Fig. 4g. Ru, O, and H atoms are indicated by green, red, and white spheres, respectively. The blue circles indicate the OH-groups resulting from the stepwise hydrogen shifts.