Supplementary Information

A Theoretical Study of an Almost Barrier-Free Water Dissociation on a Platinum (111) Surface Alloyed with Ruthenium and Molybdenum

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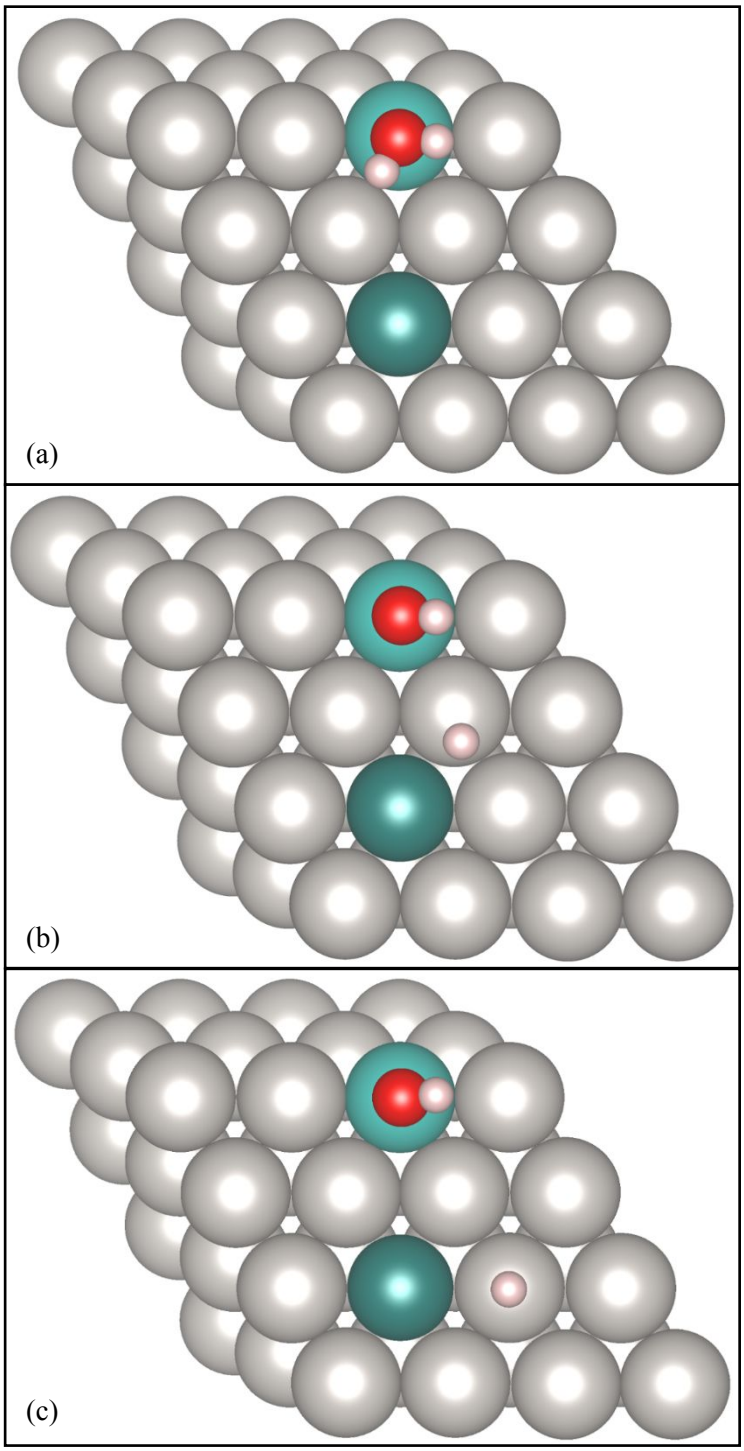

Figure S1 Atomic coordinates of the H_2O dissociation process over the Pt(111)-Ru-Mo surface for (a) initial states, (b) transition states and (c) final states. The adsorption energies of H_2O_{ad} in the initial states, H_{ad} and OH_{ad} in the transition states and H_{ad} and OH_{ad} in the final states with ZPE corrections are 1.50, 7.38 and 6.79 eV, respectively. The activation energy required to dissociate an H_2O monomer on this surface is 0.14 eV.

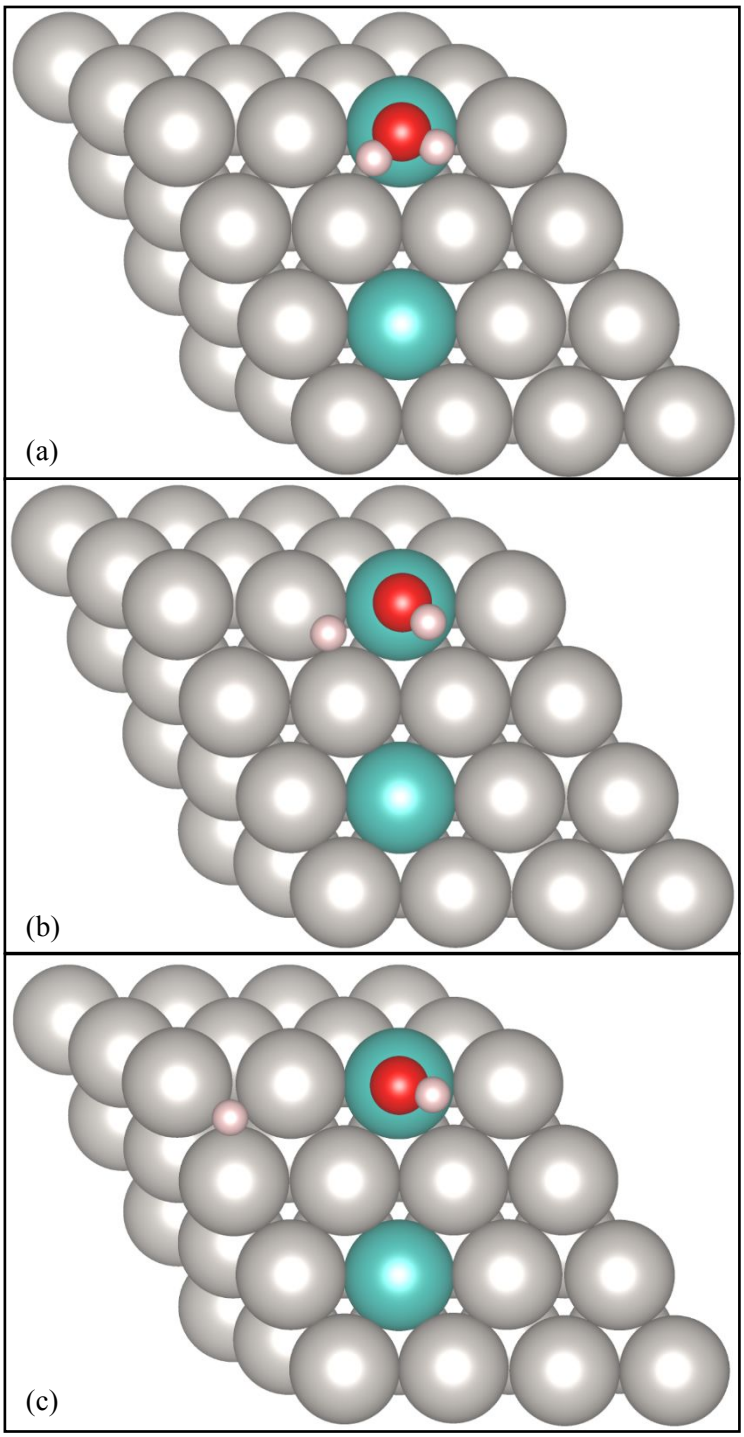

Figure S2 Atomic coordinates of the H_2O dissociation process over the Pt(111)-Mo surface for (a) initial states, (b) transition states and (c) final states. The adsorption energies of H_2O_{ad} in the initial states, H_{ad} and OH_{ad} in the transition states and H_{ad} and OH_{ad} in the final states with ZPE corrections are 1.37, 6.55 and 6.89 eV, respectively. The activation energy required to dissociate an H_2O monomer on this surface is 0.20 eV.

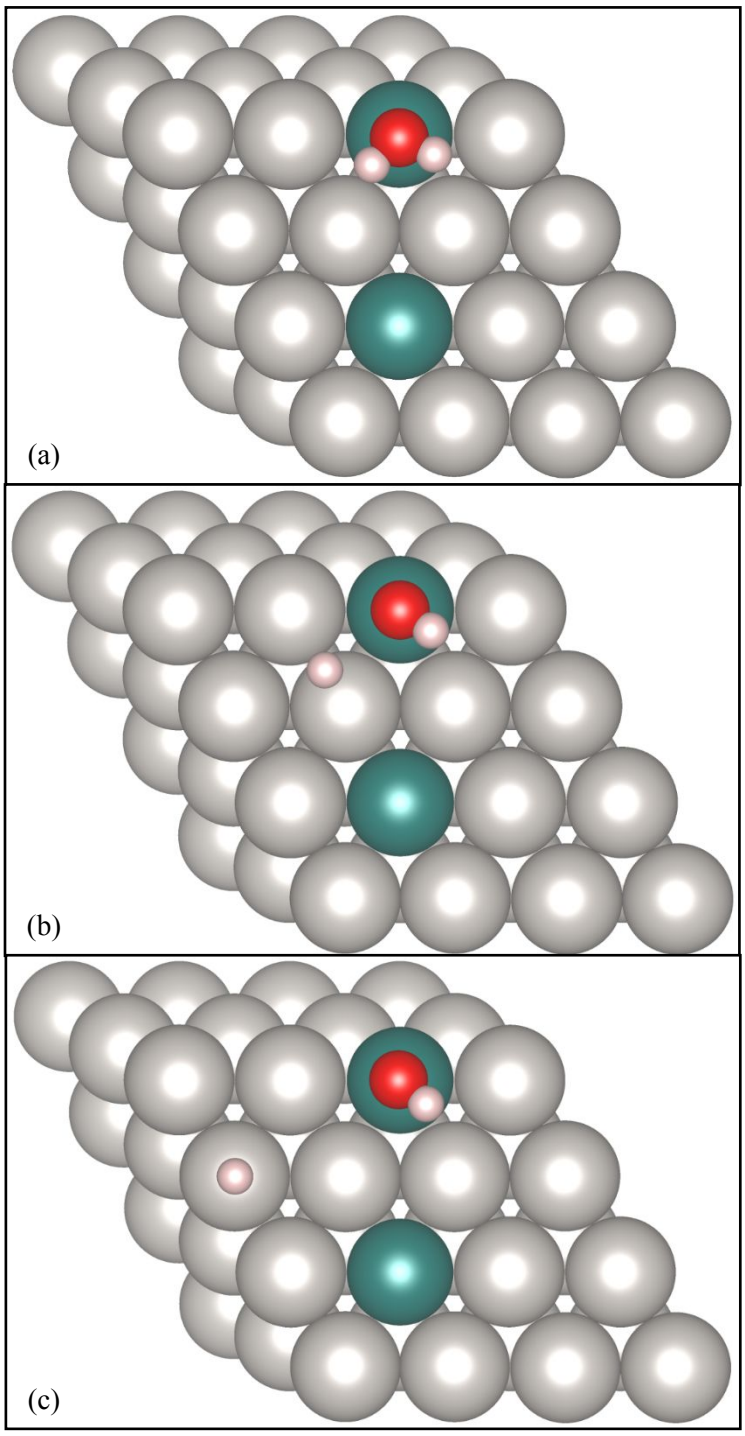

Figure S3 Atomic coordinates of the H_2O dissociation process over the Pt(111)-Ru surface for (a) initial states, (b) transition states and (c) final states. The adsorption energies of H_2O_{ad} in the initial states, H_{ad} and OH_{ad} in the transition states and H_{ad} and OH_{ad} in the final states with ZPE corrections are 1.04, 6.13 and 6.11 eV, respectively. The activation energy required to dissociate an H_2O monomer on this surface is 0.56 eV.

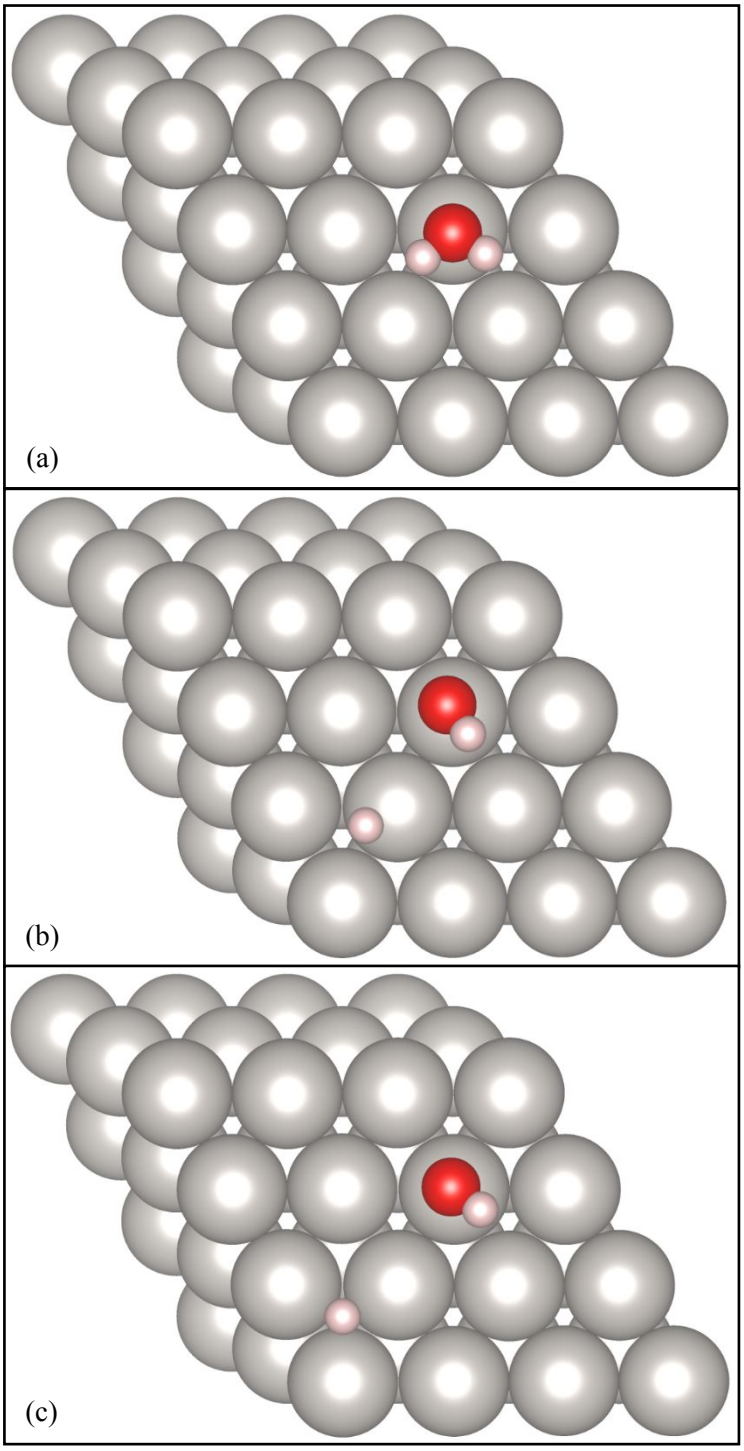

Figure S4 Atomic coordinates of the H_2O dissociation process over the pure Pt(111) surface for (a) initial states, (b) transition states and (c) final states. The adsorption energies of H_2O_{ad} in the initial states, H_{ad} and OH_{ad} in the transition states and H_{ad} and OH_{ad} in the final states with ZPE corrections are 0.30, 6.86 and 5.90 eV, respectively. The activation energy required to dissociate an H_2O monomer on this surface is 0.646 eV.