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Supporting Information

The Origin of High Electrochemical Stability of Iridium Oxides for Oxygen Evolution

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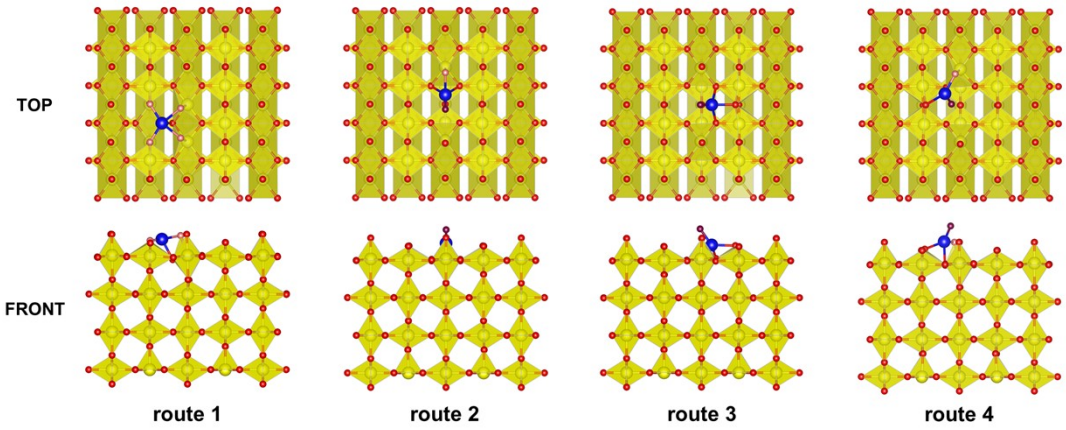

Figure S1: The surface structures of four different Ir reconstruction routes on the oxidized $IrO_2(110)$ surface.

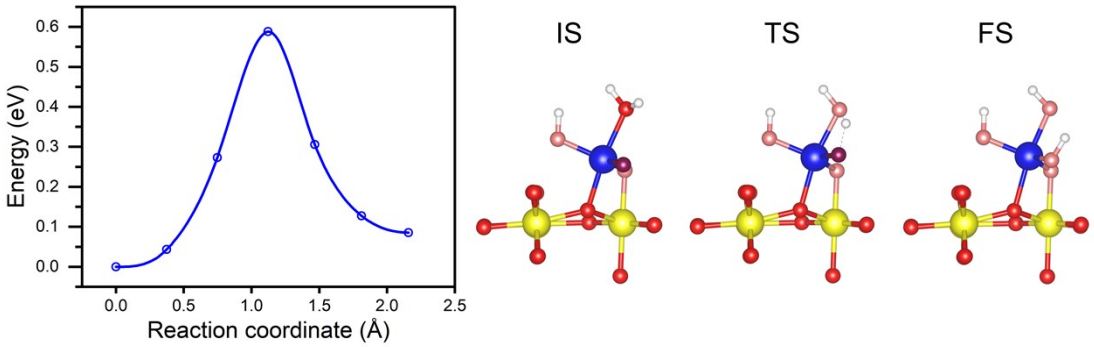

Figure S2: Calculated minimum energy path (MEP) of the process D-E' at U = 1.0 V and atomic structures of the IS, TS, and FS of the process D to E'.

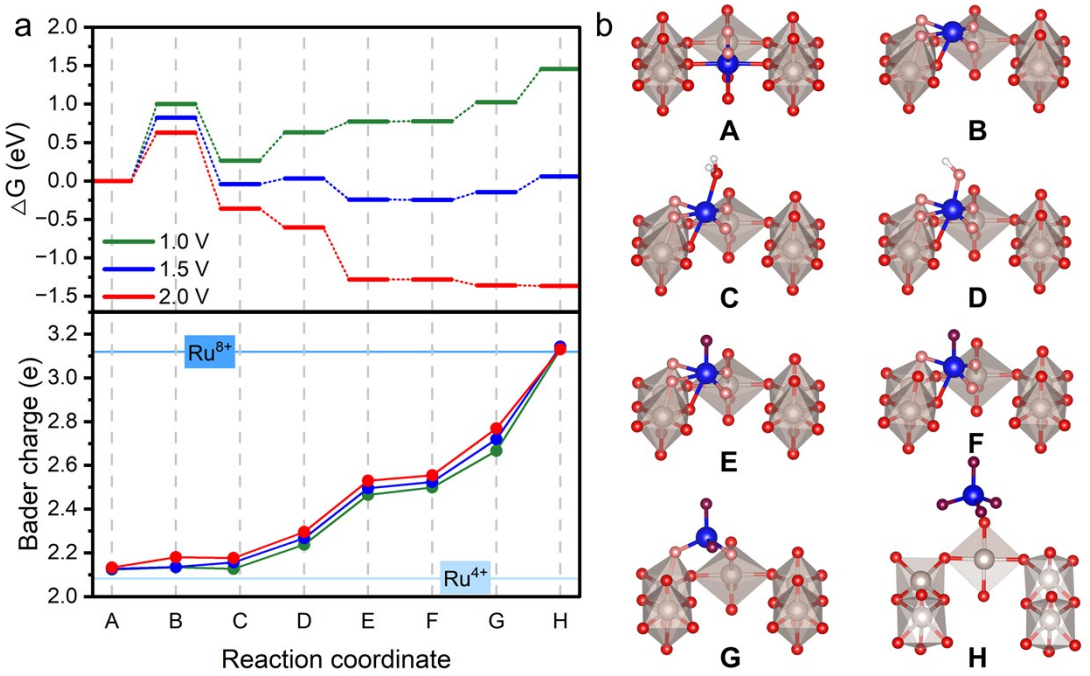

Figure S3: (a) Free energy profile of the Ru dissolution process and Bader charges of dissolving Ru at three different applied potentials. (b) The atomic structures of the dissolution intermediate. The Bader charges of Ru^{4+} in bulk RuO_2 and Ru^{8+} in bulk RuO_4 are used to serve as the reference for assigning the valence states of the dissolving Ru.

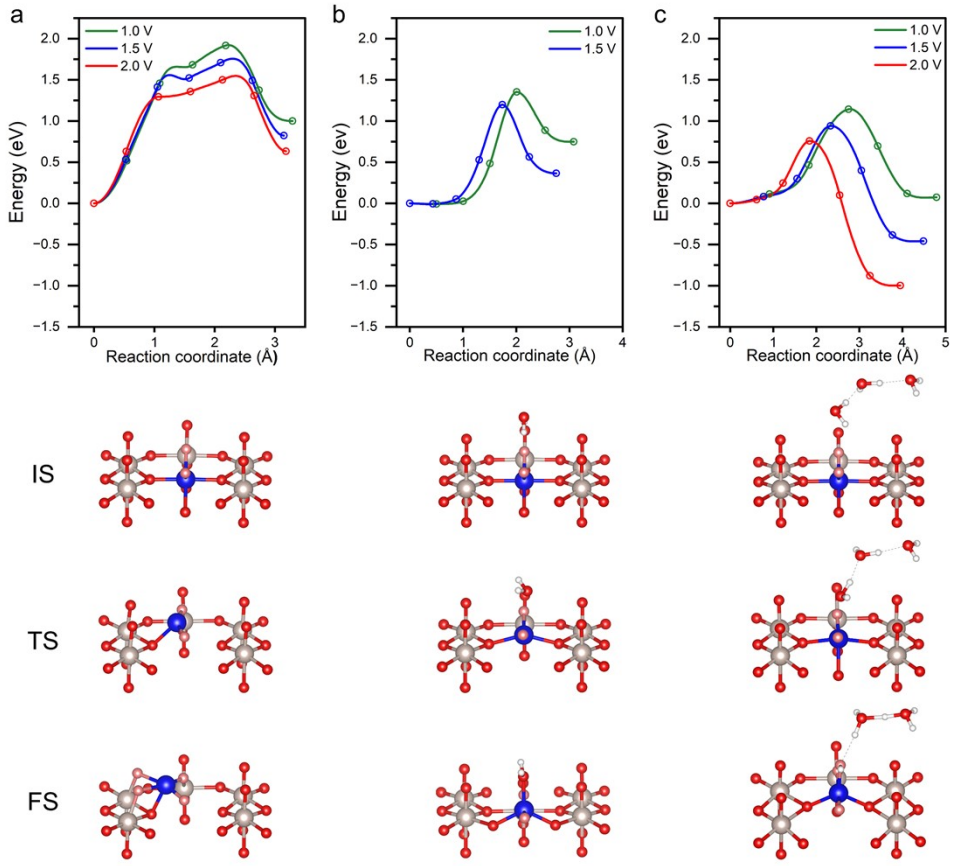

Figure S4: Potential-dependent MEPs and the transition state structure for the Ru reconstruction via (a) the direct Ru reconstruction, (b) the water adsorption induced Ru reconstruction, (c) the water oxidation induced Ru reconstruction.

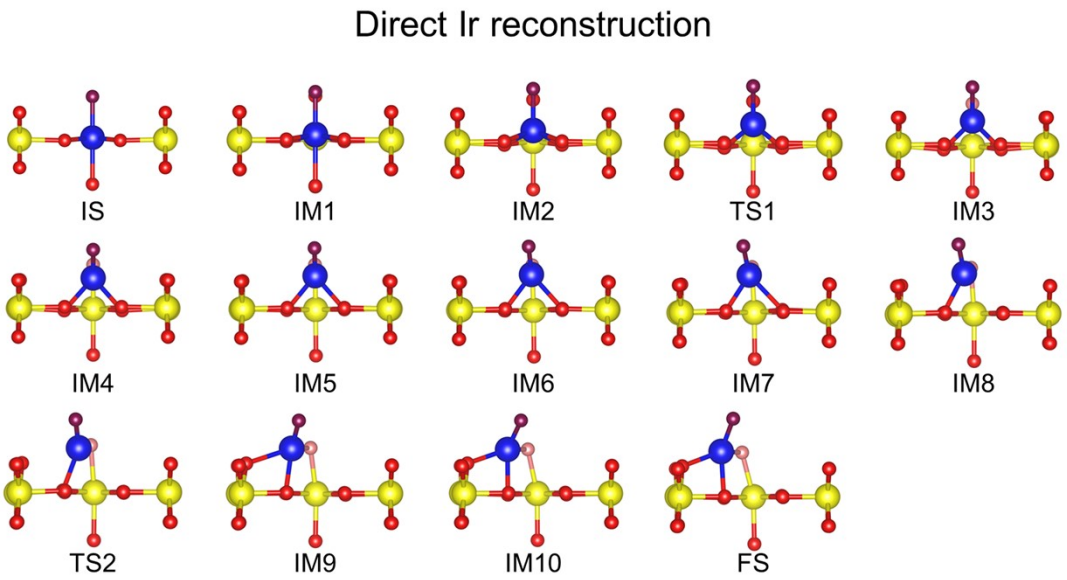

Figure S5: Image structures of the eNEB calculations for the direct Ir reconstruction pathway at U = 1.5 V.

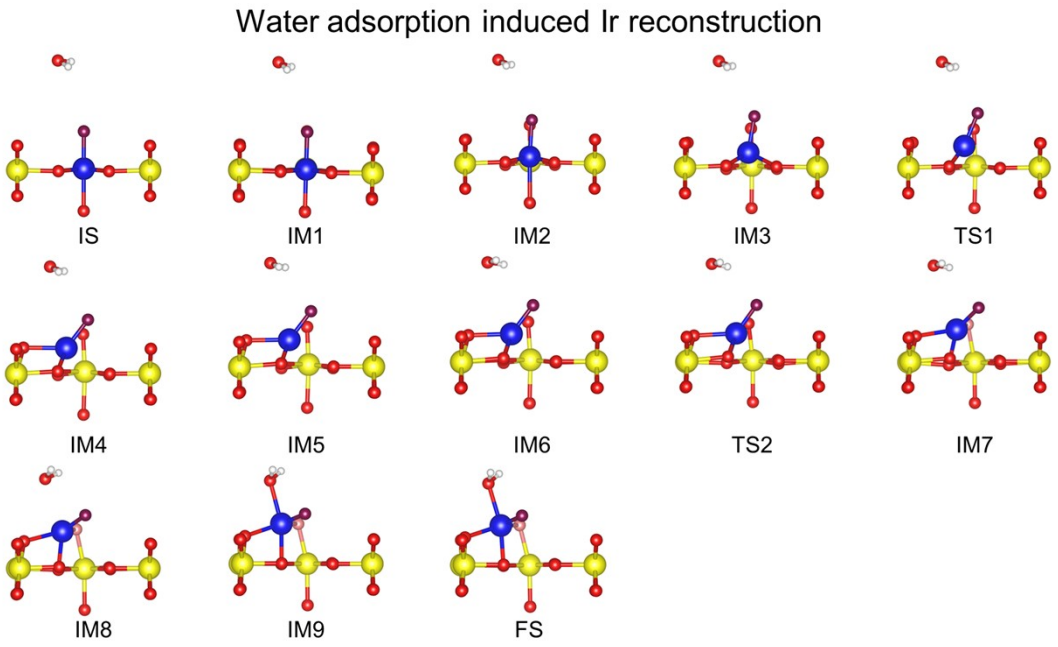

Figure S6: Image structures of the eNEB calculations for the water adsorption induced Ir reconstruction pathway at U = 1.5 V.

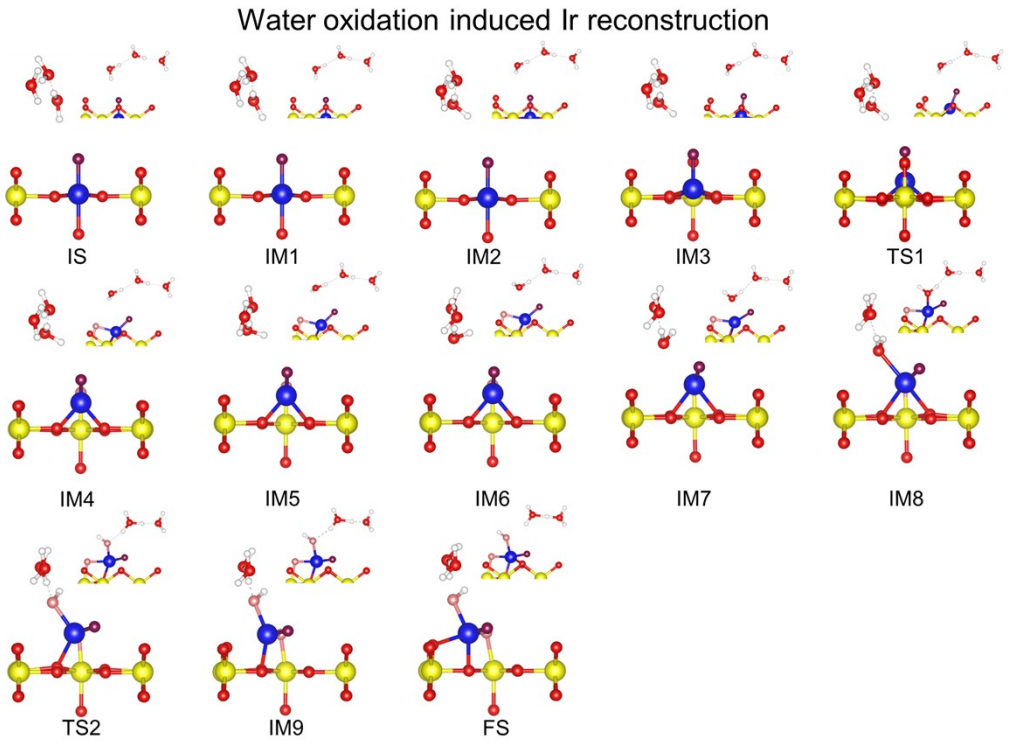

Figure S7: Image structures of the eNEB calculations for the water oxidation induced Ir reconstruction pathway at U = 1.5 V.

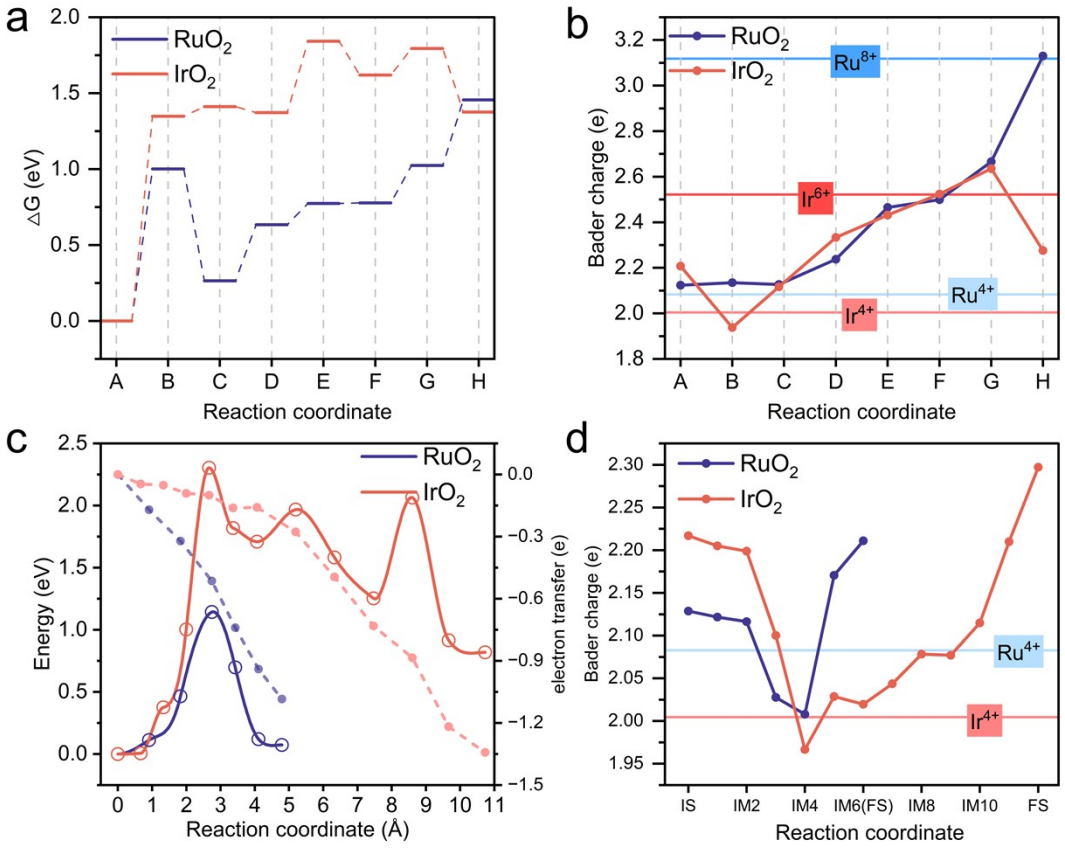

Figure S8: Comparison between Ir and Ru reconstruction. (a) Free energy diagrams of Ir and Ru dissolution processes at U = 1.0 V. (b) Evolution of Bader charges of the dissolving Ir and Ru along the dissolution process. (c) Minimum energy paths (MEPs) and net electron transfer of Ru and Ir dissolution at U = 1.0 V via the water oxidation induced mechanism. (d) Variation of Bader changes of the reconstructing Ru and Ir along the MEPs in (c).

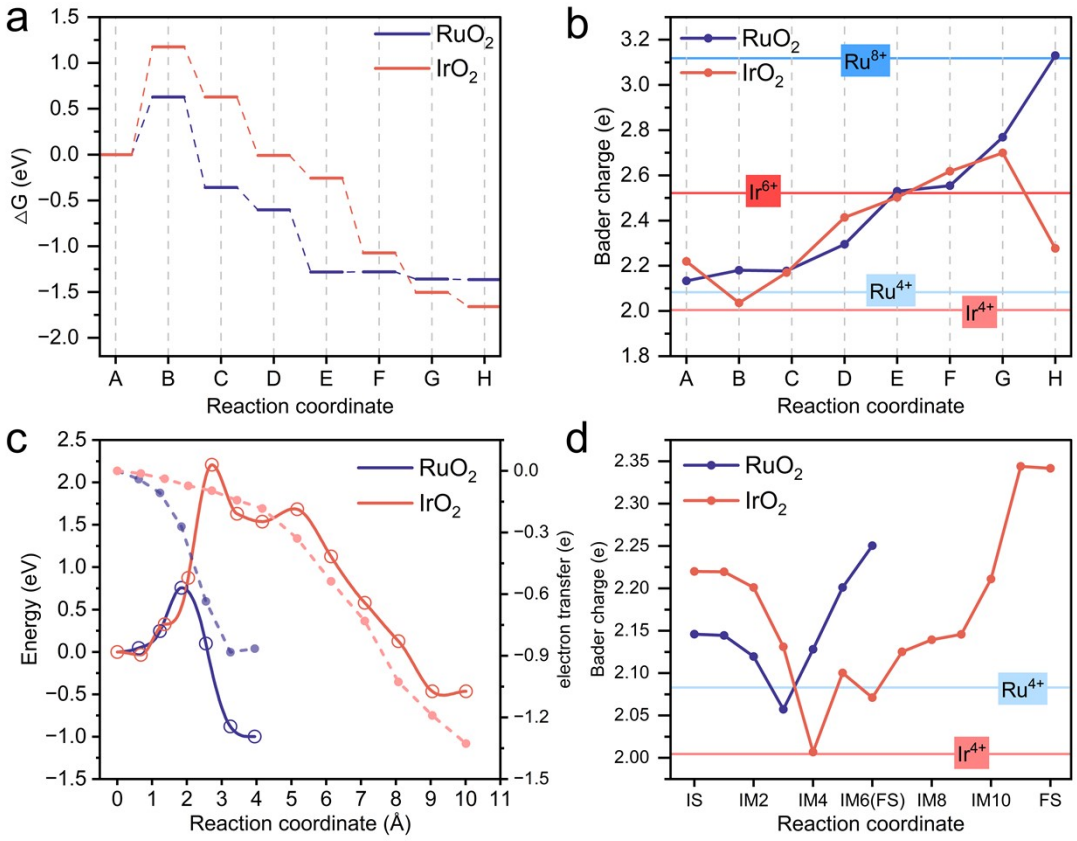

Figure S9: Comparison between Ir and Ru reconstruction. (a) Free energy diagrams of Ir and Ru dissolution processes at U = 2.0 V. (b) Evolution of Bader charges of the dissolving Ir and Ru along the dissolution process. (c) Minimum energy paths (MEPs) and net electron transfer of Ru and Ir dissolution at U = 2.0 V via the water oxidation induced mechanism. (d) Variation of Bader changes of the reconstructing Ru and Ir along the MEPs in (c).