Supporting Information

Understanding the Catalysis of Noble Metals in Reduction of Iron Oxide by Hydrogen: Insights from DFT Calculations

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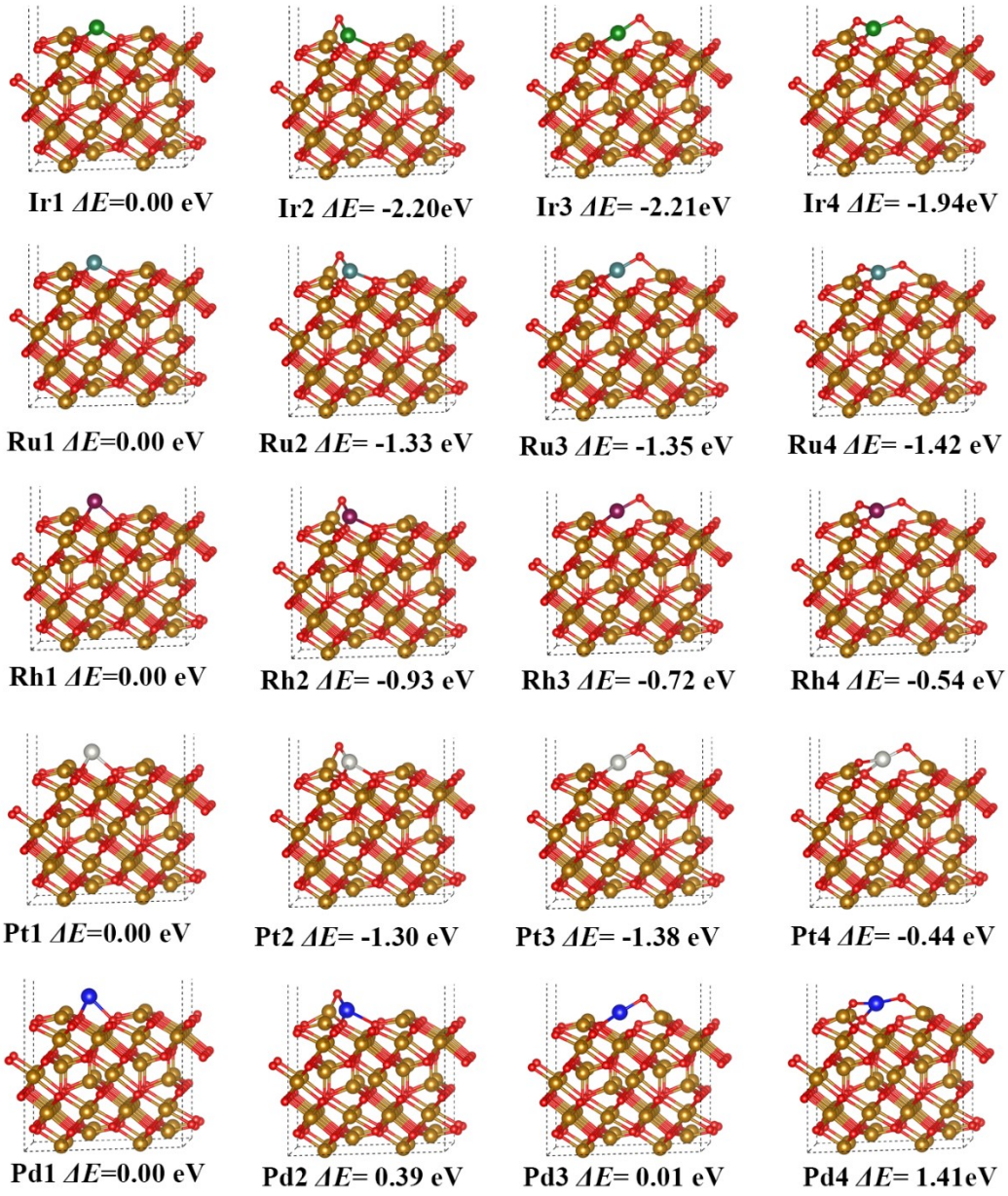

Figure S1. Optimized structures along with the relative energies for different noble metal (NM) on the substrate.

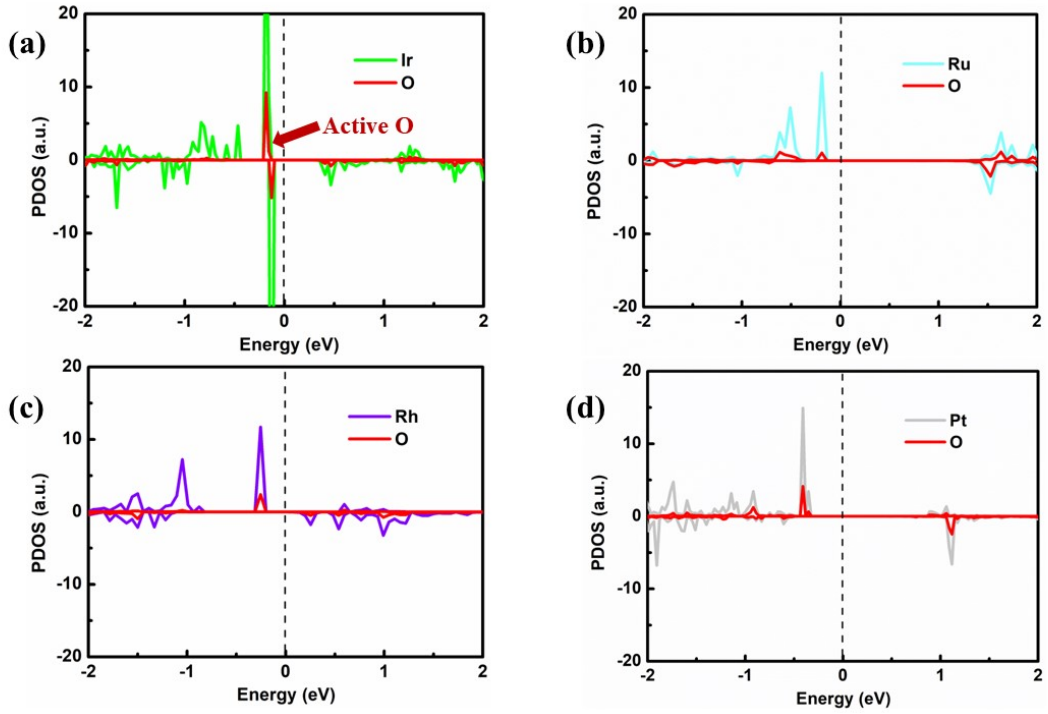

Figure S2. Projected density of states of noble metals and active oxygen after introducing noble metals in Fe_3O_4: (a) Ir/Fe_3O_4, (b) Ru/Fe_3O_4, (c) Rh/Fe_3O_4, (d) Pt/Fe_3O_4. The Fermi level is set to be zero with a dashed line as a guide.

Table S1. DFT calculated d-band centers (eV) of different noble metals introducing into the Fe_3O_4 (111) surface; the reference energy level is vacuum.

	Ir	Ru	Rh	Pt	Pd
d-band center	-3.49	-3.61	-3.87	-4.62	-3.21
ΔQ (e)	0.64	1.12	0.63	0.53	0.52

Table S2. DFT calculated energy of HOMO and LUMO for free hydrogen molecules; the reference energy level is vacuum.

Free H_2 molecule	
HOMO (eV)	-10.33
LUMO (eV)	-0.03

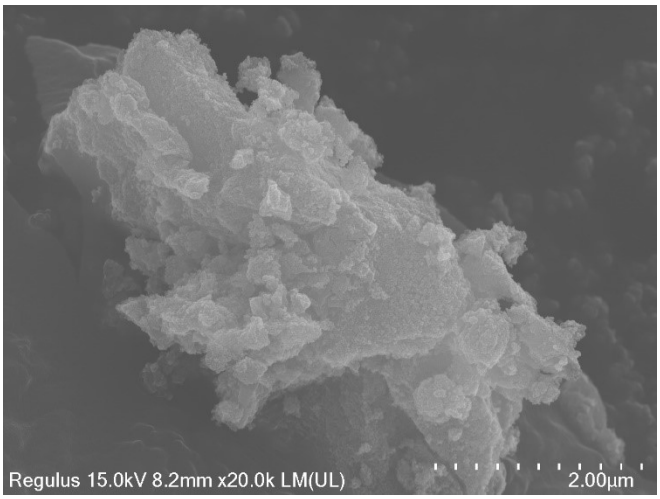

Figure S3. SEM image of as prepared pristine Fe_2O_3/ZrO_2.

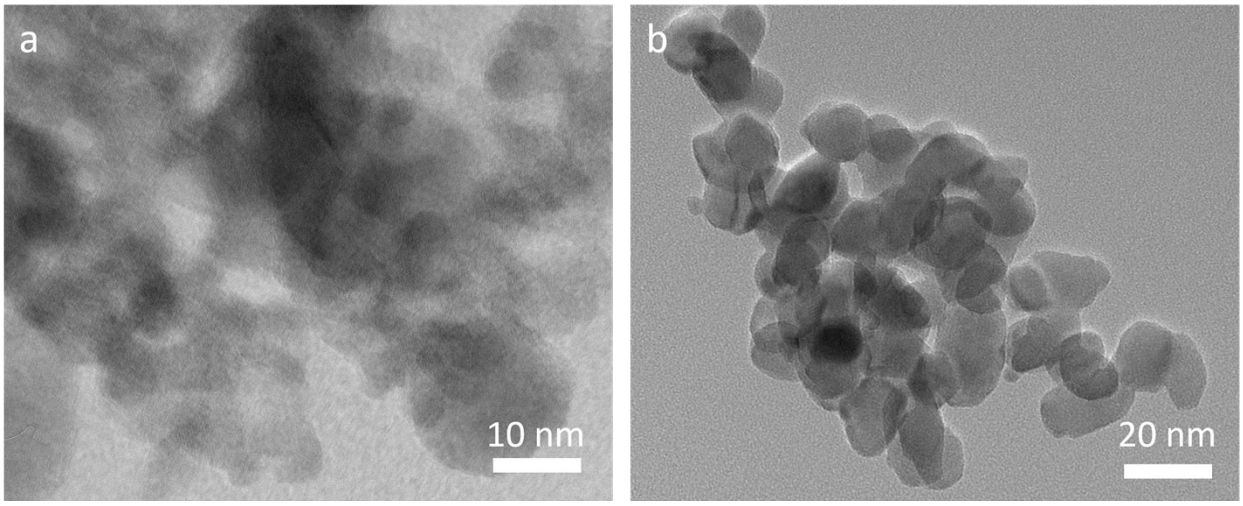

Figure S4. TEM images of (a) pristine Fe_2O_3/ZrO_2, (b) Ir-Fe_2O_3/ZrO_2.

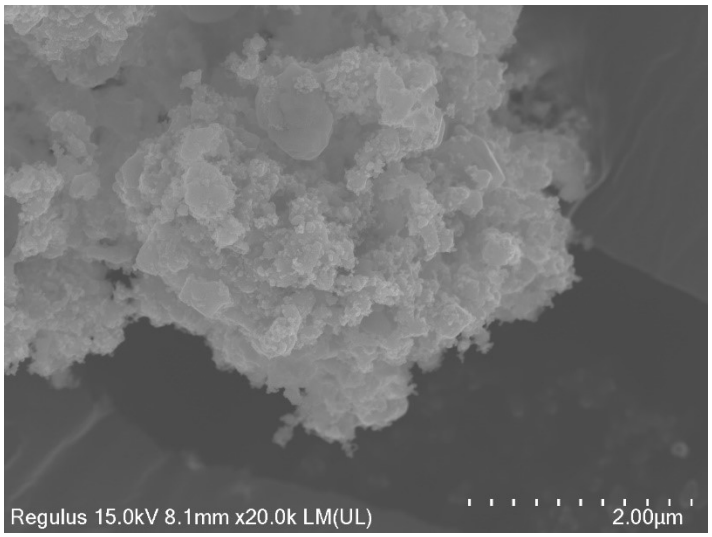

Figure S5. SEM image of Ir-Fe_2O_3/ZrO_2 after 100 cycles testing.

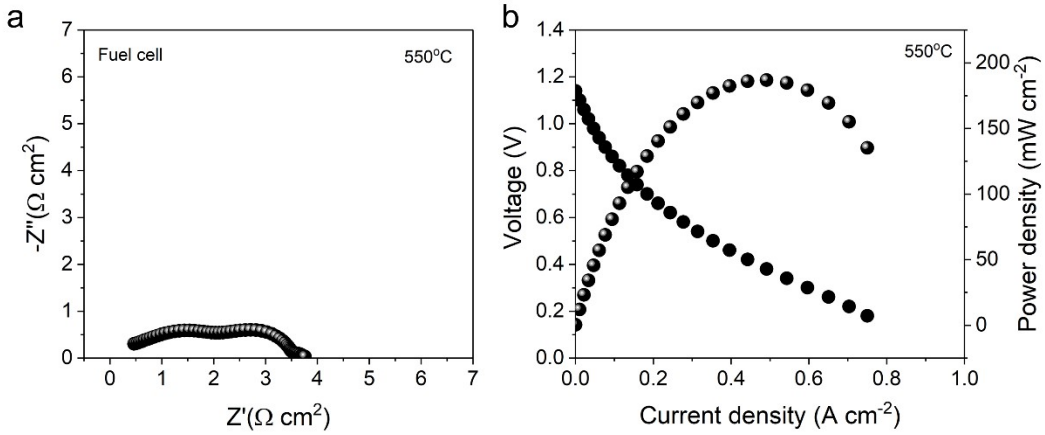

Figure S6. (a) EIS spectrum of reversible solid oxide fuel cell; (b) I-V and corresponding I-P curves of reversible solid oxide fuel cell.

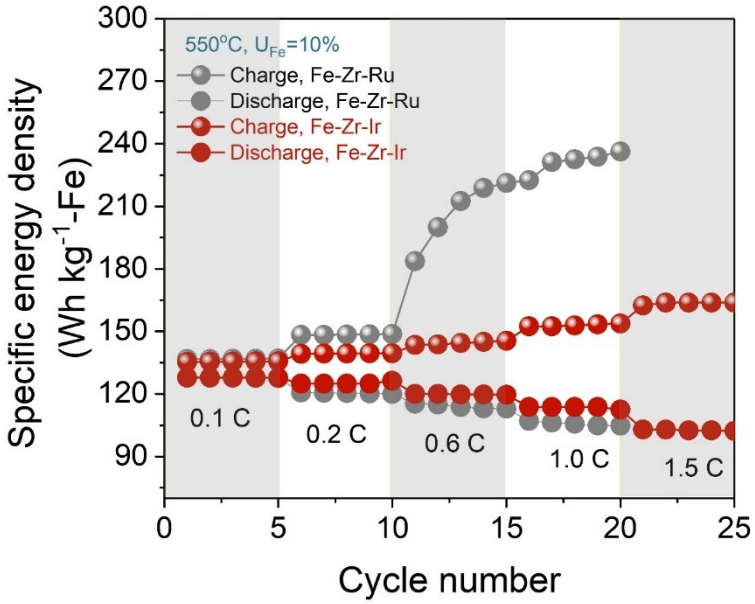

Figure S7. Comparison of specific energy density at different current densities for Ir-and Ru-Fe_2O_3/ZrO_2 energy storage materials.

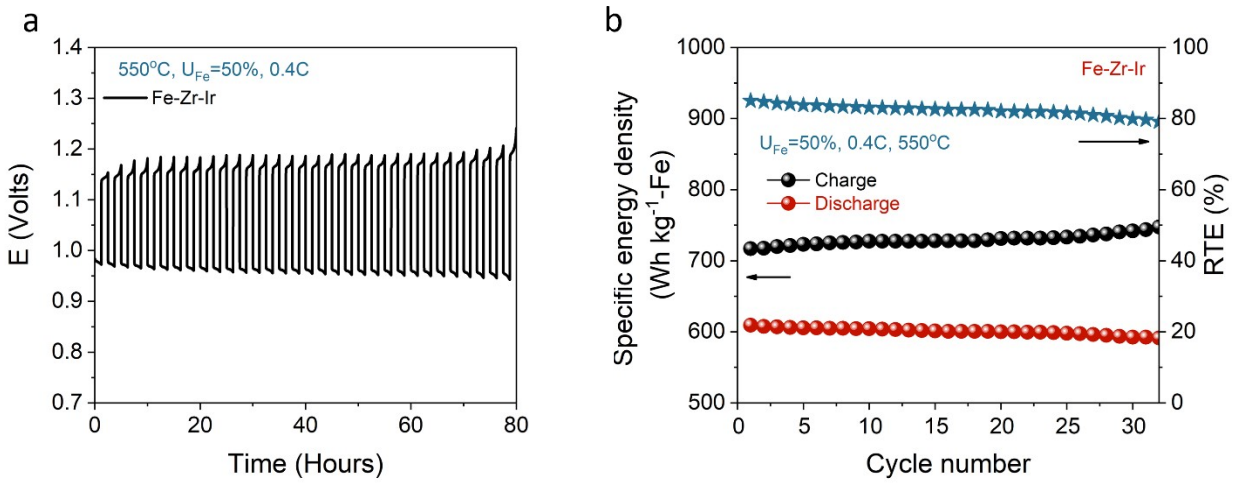

Figure S8. Cycling performance of SOIAB with 0.4C (20mA/cm^2) and U_{Fe}=50%: (a) voltage profiles; (b) the corresponding specific energy density and round-trip efficiency.

Table S3. Valence electron configurations of different metals and O adopted in this work.

Element	Fe	Ir	Pt	Ru_pv	Rh_pv	Pd	O
Valence electron	$3d^74s^1$	$6s^15d^8$	$6s^15d^9$	$4p^65s^14d^7$	$4p^65s^14d^8$	$5s^14d^9$	$2s^22p^4$
Number	8	9	10	14	15	10	6