Supporting information

Insight into the effect of electronegativity on H_2 activation for CO_2 hydrogenation: Four transition metal cases from a DFT study

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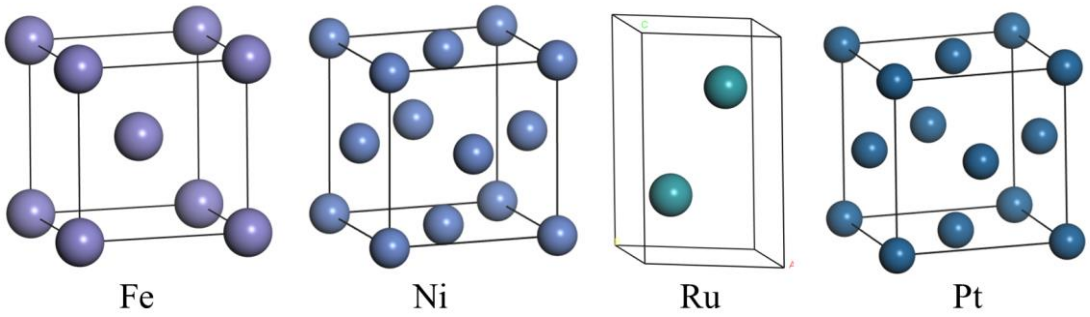

Figure S1. Crystal cells of Fe, Ni, Ru and Pt.

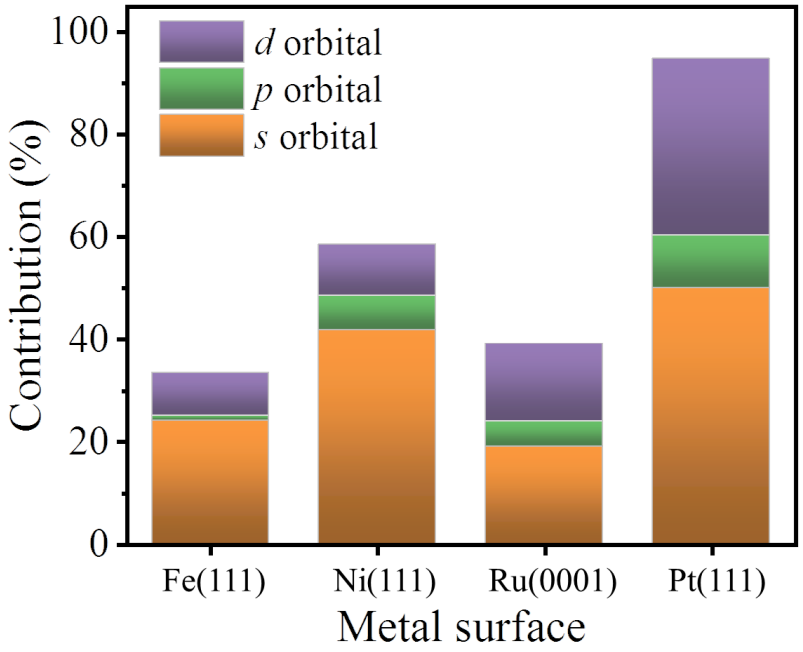

Figure S2. Orbital contribution for H_2 dissociation on Fe(111), Ni(111), Ru(0001) and Pt(111).

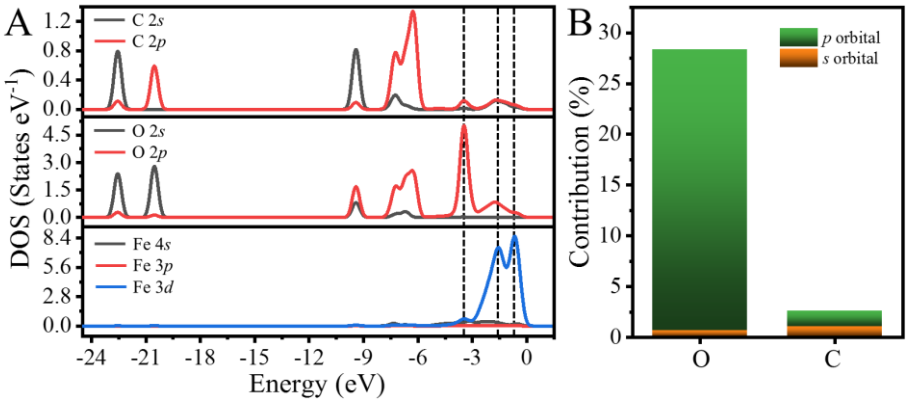

Figure S3. (A) Partial density of states (PDOS) for CO_2 adsorption on Fe(111), and (B) the corresponding orbital contribution of CO_2 for overlapping with Fe 3*d* orbital.

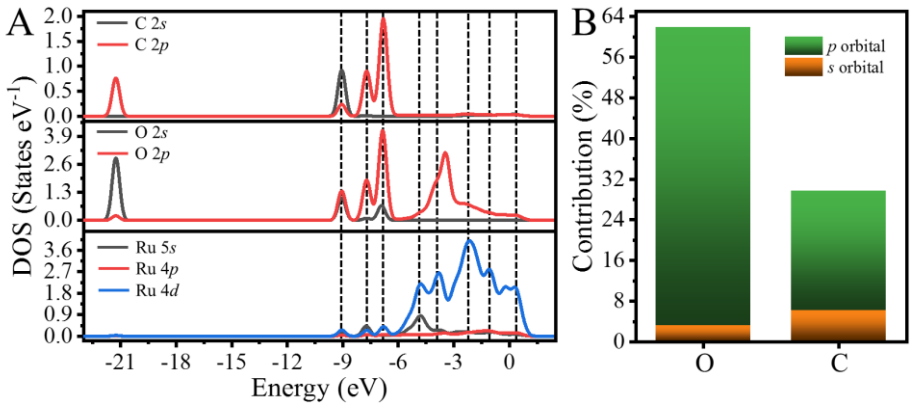

Figure S4. Partial density of states (PDOS) for CO_2 adsorption on Ru(0001), and (B) the corresponding orbital contribution of CO_2 for overlapping with Ru 4*d* orbital.

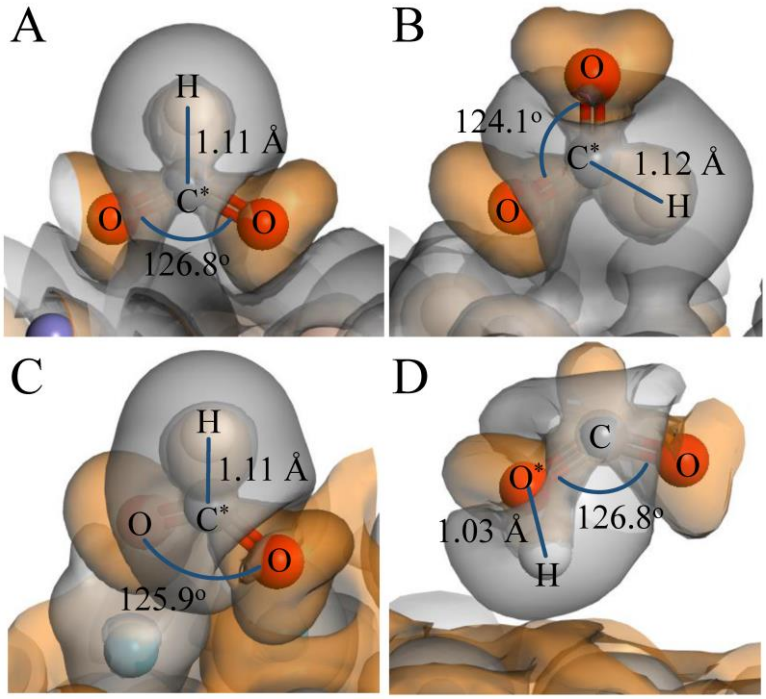

Figure S5. Deformation charge density for free adsorption of the activated CO_2 molecule on the H-assisted (A) Fe(111), (B) Ni(111), (C) Ru(0001) and (D) Pt(111).

Table S1

Construction information for Fe, Ni, Ru and Pt bulk metal and supercell after optimization.

Transition metal	Fe	Ni	Ru	Pt
Supercell	Fe(111)	Ni(111)	Ru(0001)	Pt(111)
Supercell size	(2 × 2 × 6)	(3 × 3 × 4)	(3 × 3 × 5)	(3 × 3 × 5)
Vacuum space	20 Å	20 Å	20 Å	20 Å
Atomic number	24	36	45	45
Lattice parameter of bulk metal	a = 2.8664 Å	a = 3.5240 Å	a = 2.7058 Å c = 4.2816 Å	a = 3.9239 Å
Lattice parameter of supercell	a = b = 8.1074 Å c = 24.1373 Å	a = b = 7.4755 Å c = 26.1037 Å	a = 8.1174 Å b = 8.1174 Å c = 28.5632 Å	a = b = 8.3238 Å c = 29.0619 Å