Supporting information for:

Rational design of metal-single-atom decorated $CaTaO_2N$ as multifunctional photocatalysts for water splitting and CO_2 reduction

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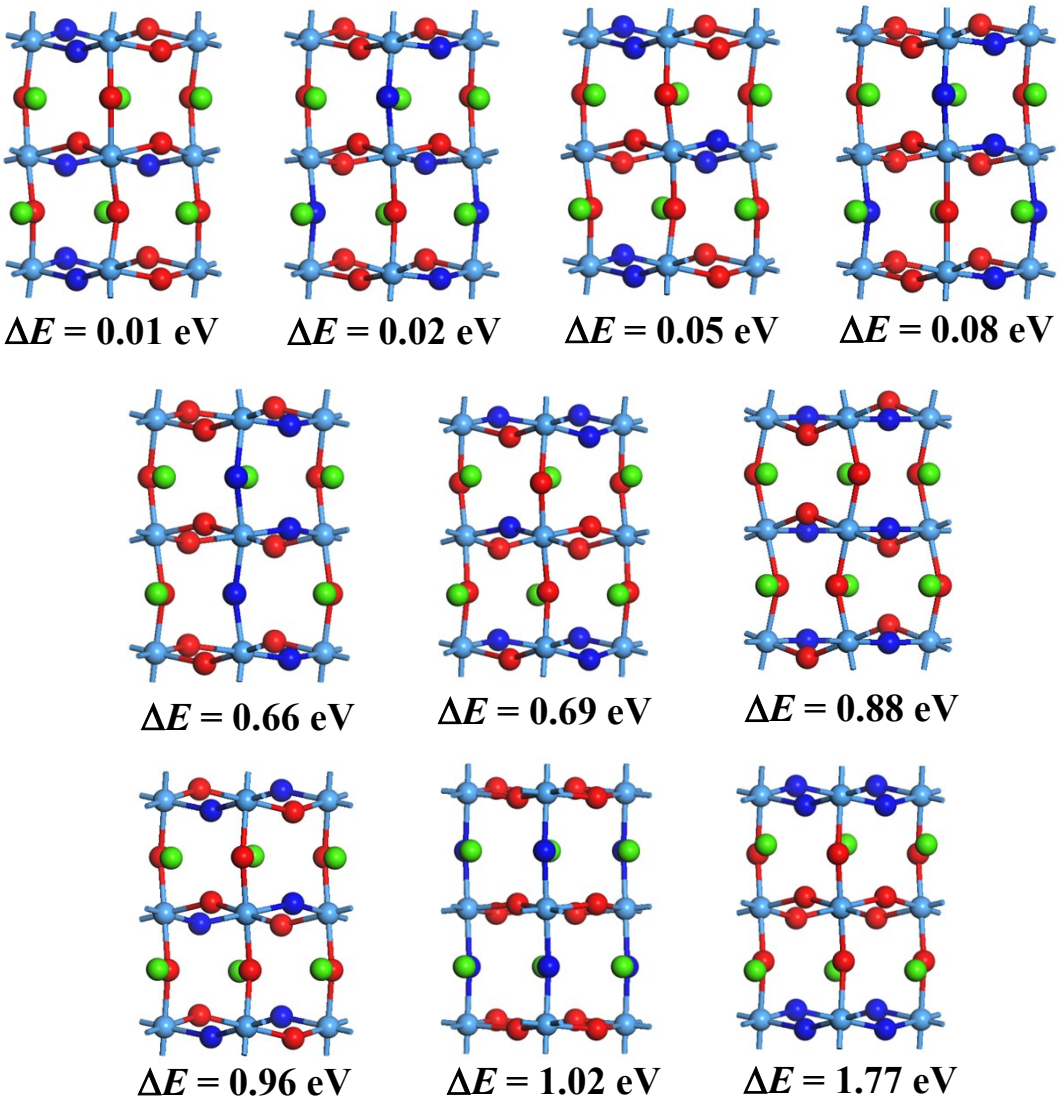

Fig. S1 Optimized structures with higher energies relative to the most stable structure, along with the relative energy ΔE.

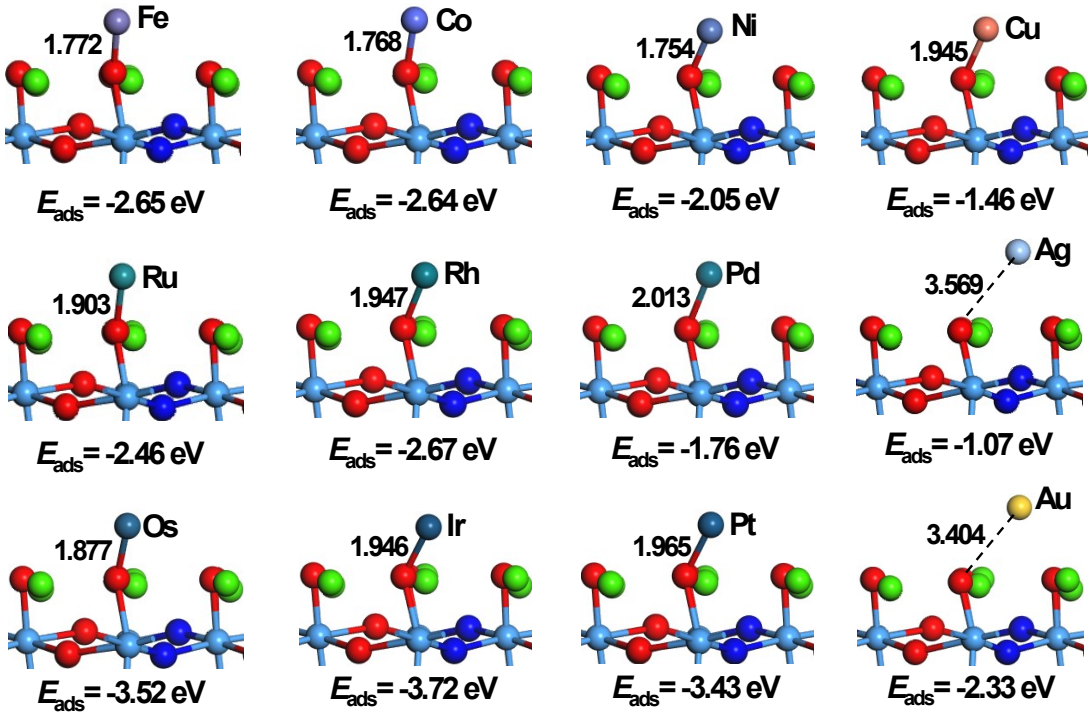

Fig. S2 Local geometries of optimized adsorption configurations for single metal atoms on the CaO-terminated $CaTaO_2N$(010) surface. Bond lengths of newly formed bonds are indicated in the figures, along with the corresponding adsorption energies.

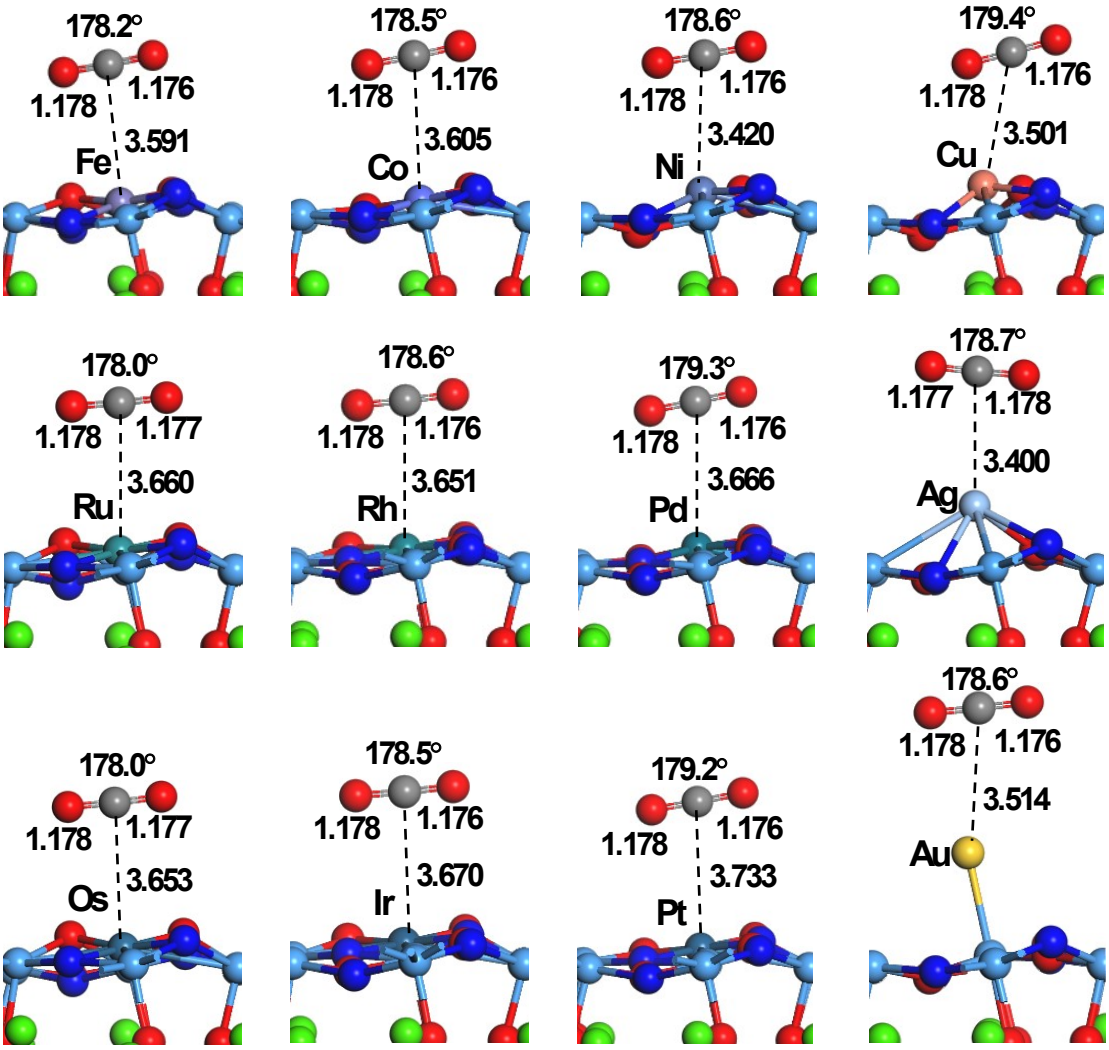

Fig. S3 Optimized adsorption structures of linear *CO_2 on the modeled surfaces, with key structural parameters.

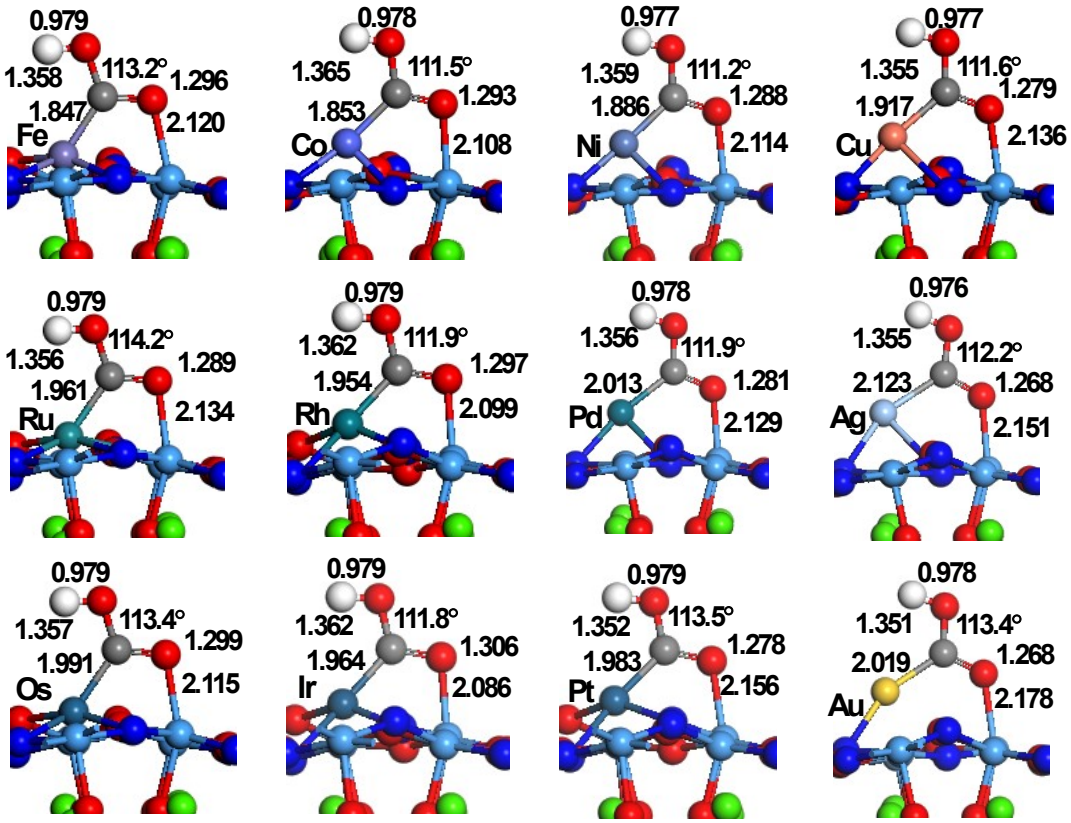

Fig. S4 Optimized adsorption structures of linear HOOC* on the modeled surfaces, with key structural parameters.

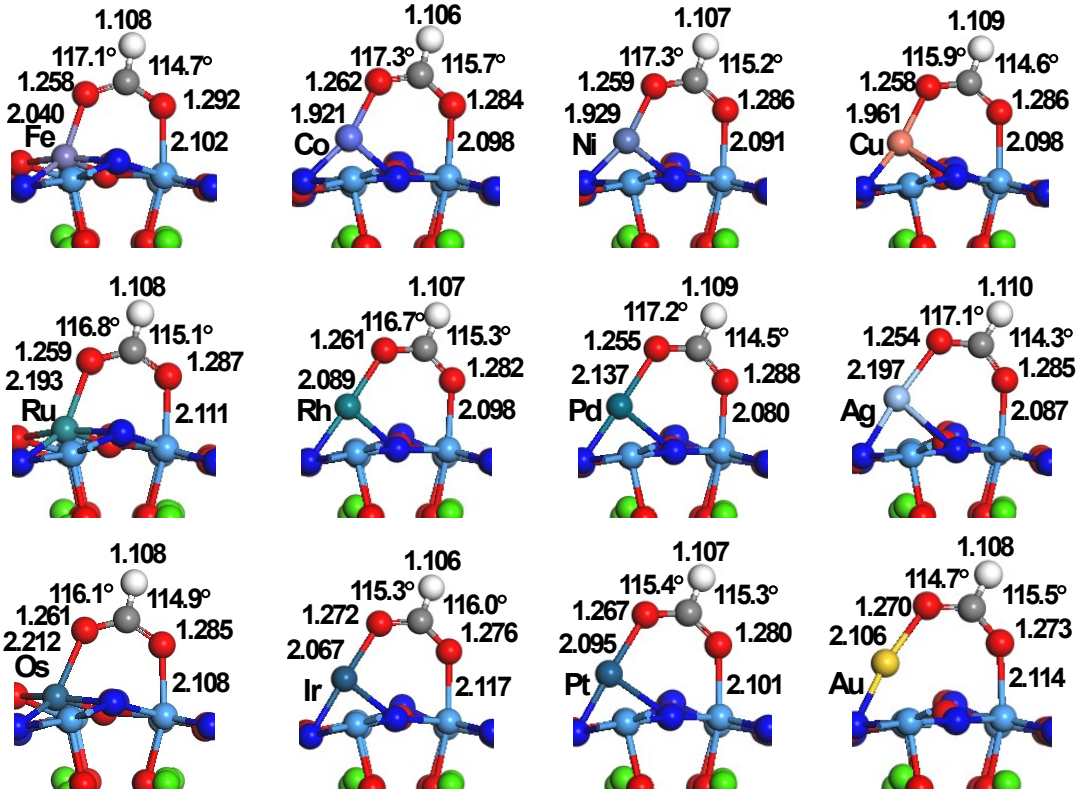

Fig. S5 Optimized adsorption structures of linear OHCO* on the modeled surfaces, with key structural parameters.