

Supplementary information

Theoretical study of CO₂ adsorption on Pt

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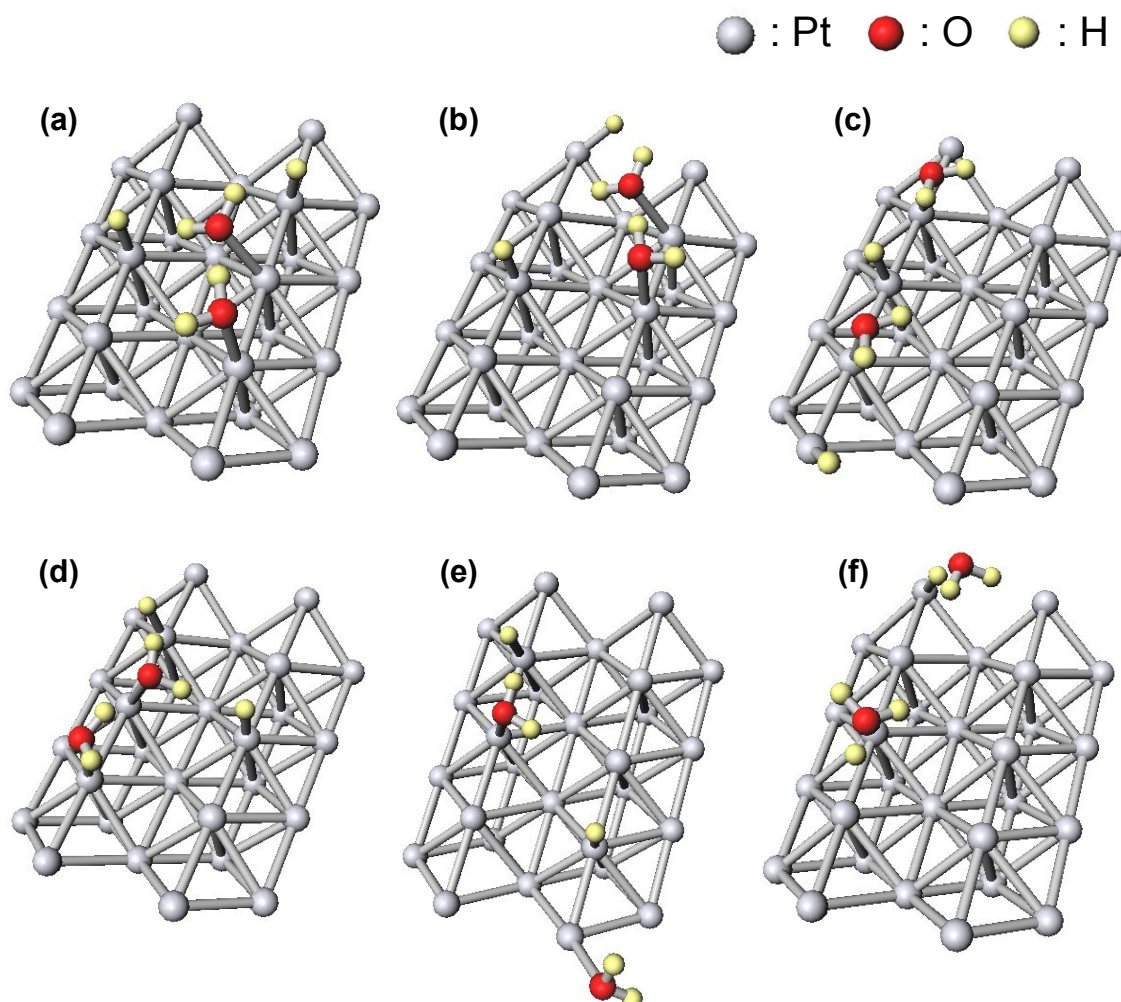


Fig. S1 The calculation results of the adsorption structure in which two molecules of H₃O⁺ are adsorbed to a Pt (110) cluster.

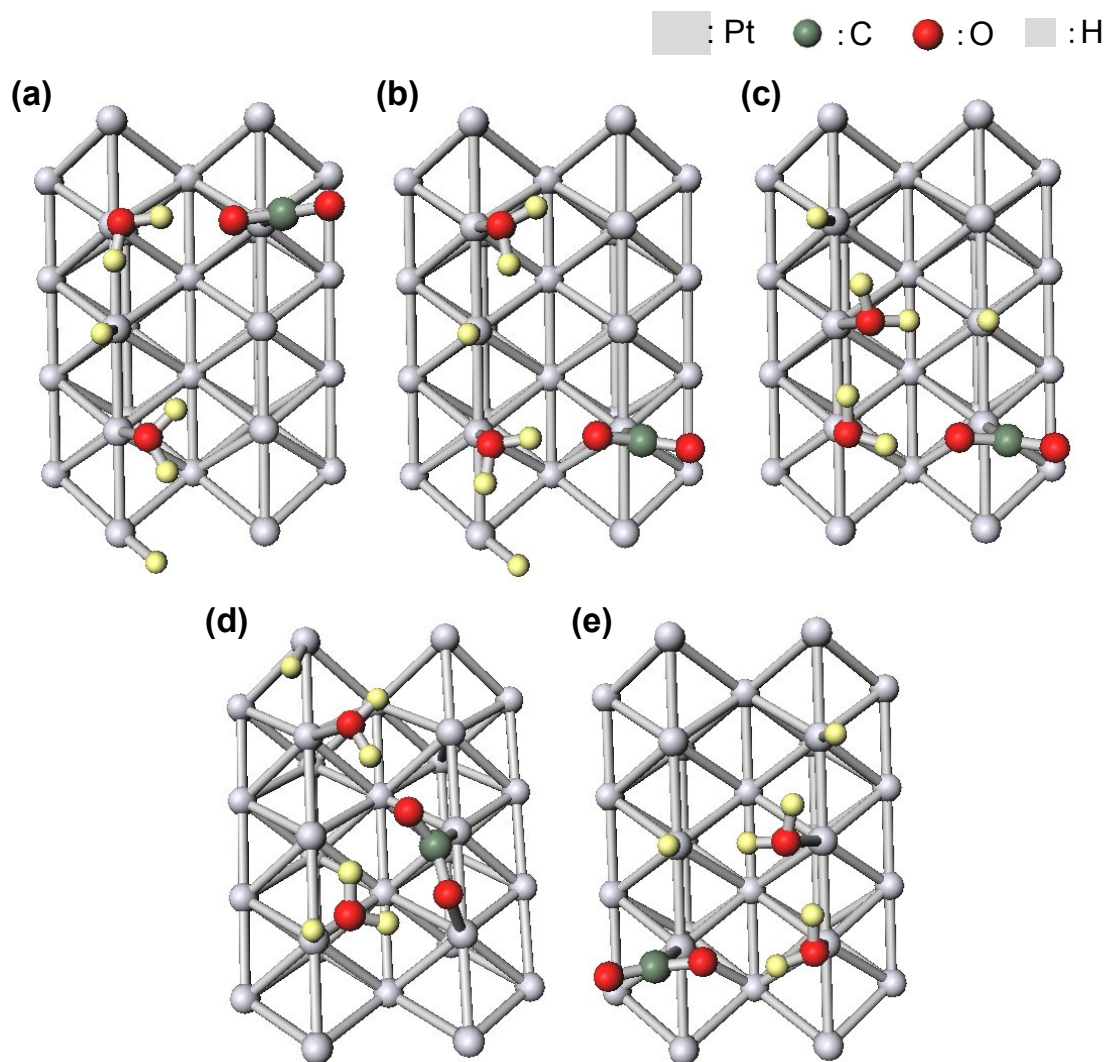


Fig. S2 The calculation results of the CO₂-adsorbed state, except for Fig. 3a.

Table S1 ΔG_{ads} values for all six CO₂-adsorbed states.

	$\Delta G_{\text{ads}} / \text{kJ mol}^{-1}$
Fig. 3a	-160
Fig. S2a	-153
Fig. S2b	-155
Fig. S2c	-159
Fig. S2d	-147
Fig. S2e	-157

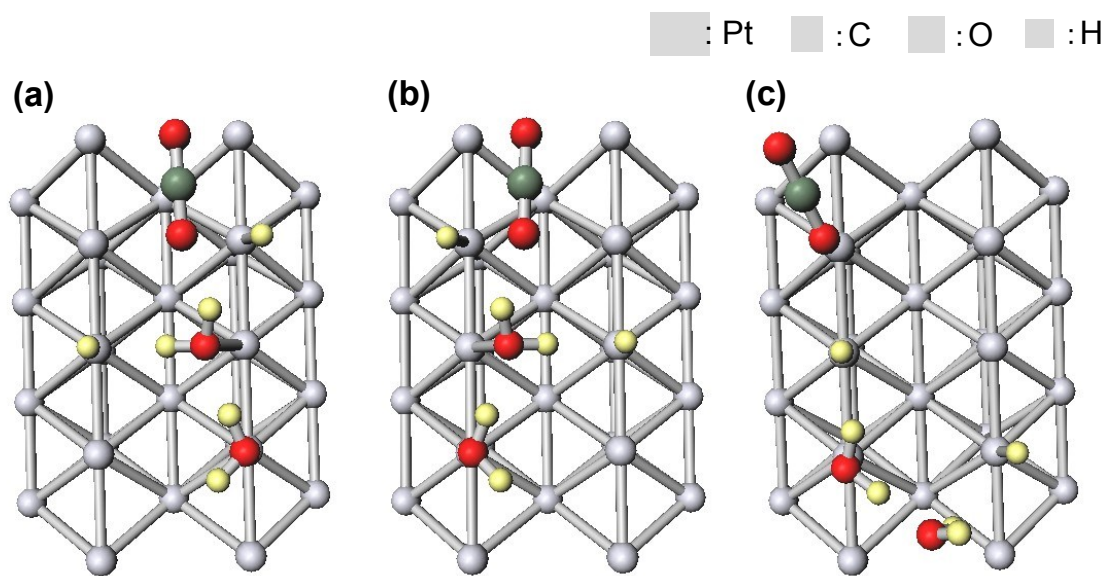


Fig. S3 The calculation results of the CO₂ non-adsorbed state.