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C-O bond activation and splitting behaviors of CO_2 on 4H-SiC surface: a DFT study

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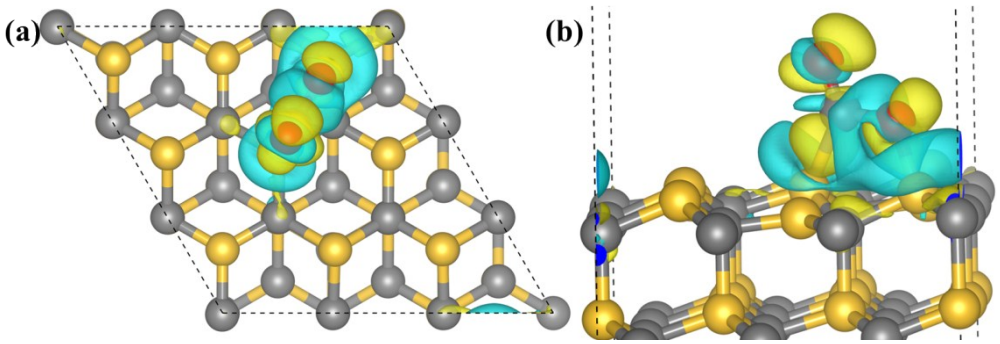

Fig. S1 The isosurface of the difference charge density with the isovalue of 0.0028 Å^{-3} and the blue (yellow) wireframes denote loss (gain) of electrons. Red, gray and yellow balls represent O C and Si atoms, respectively.

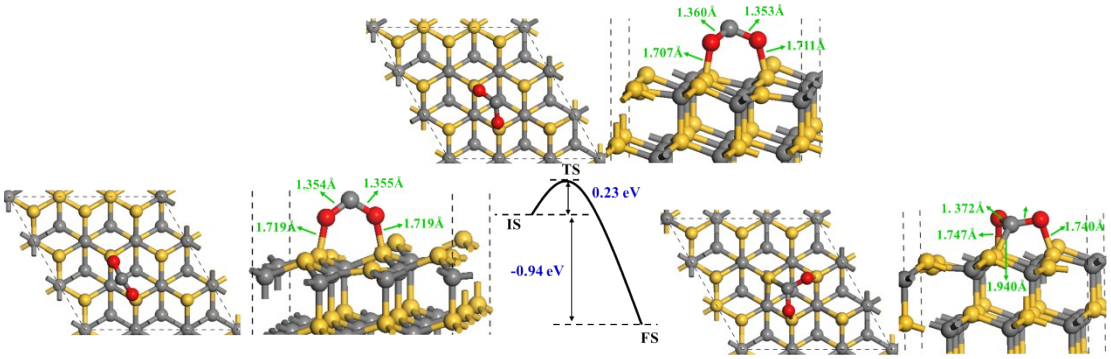

Fig. S2 The minimum energy path for transformation from the adsorption configuration in Fig. 2(a) to that in Fig. 2(d). Gray, red and yellow balls represent C, O, and Si atoms, respectively. The bond lengths in transition state (TS) are close to those in initial structure, suggesting that the TS is more reactant-like than product-like.

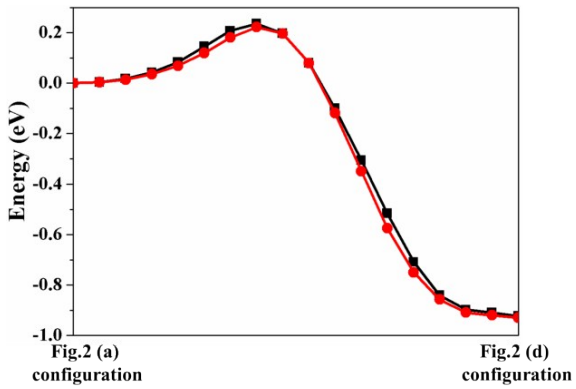

Fig. S3 The transformation paths from Fig. 2(a) to (d) with (in red) and without (in black) vdw correction.

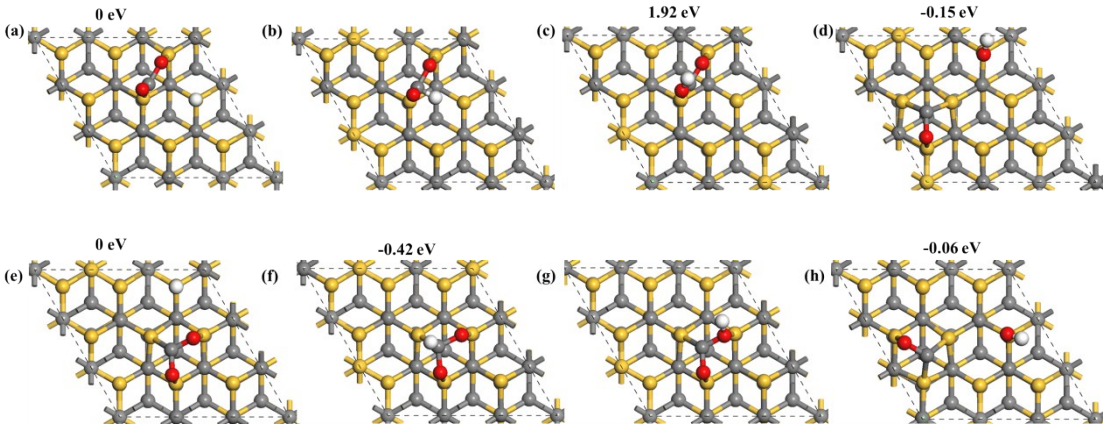

Fig. S4 Four possible structures of CO_2+H co-adsorption, COOH group, HCOO group and CO+OH co-adsorption on SiC(0001) surface: (a)-(d) are for $CO_2^{\delta-}$ configuration in the case of H atom; (e)-(h) are for tridentate CO_2 in the case of H atom. Gray, red, yellow and H balls represent C, O, Si and H atoms, respectively. The energies are relative to those of CO_2+H co-adsorption states. (a), (c), (d), (e), (f), and (h) are optimized structures, while (b) and (g) are unoptimized structures. After fully optimization, structure (b) turns into structure (a) and structure (g) become structure (e).

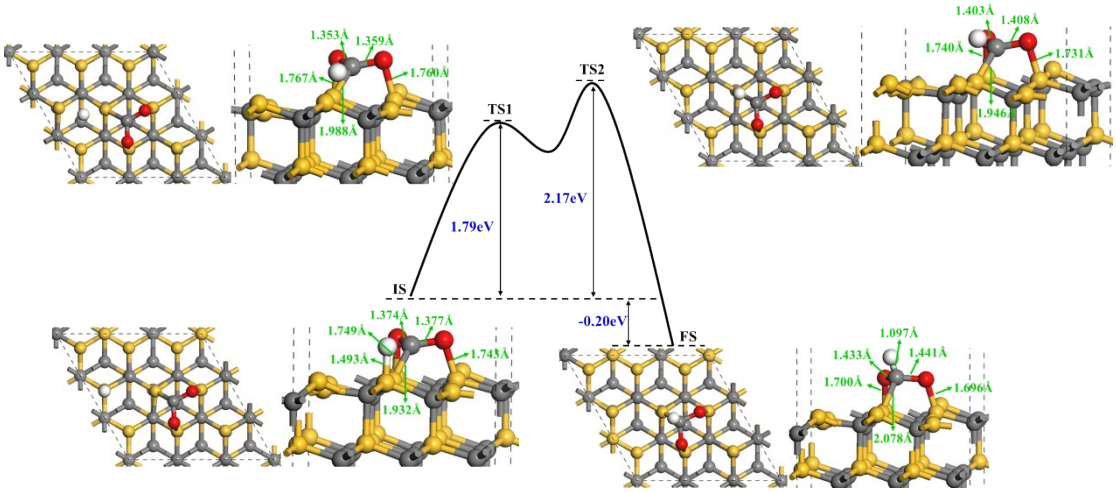

Fig. S5 The minimum energy path for transformation from CO_2+H co-adsorption to OCHO group. Gary, red, yellow, and white balls represent C, O, Si and H atoms, respectively.

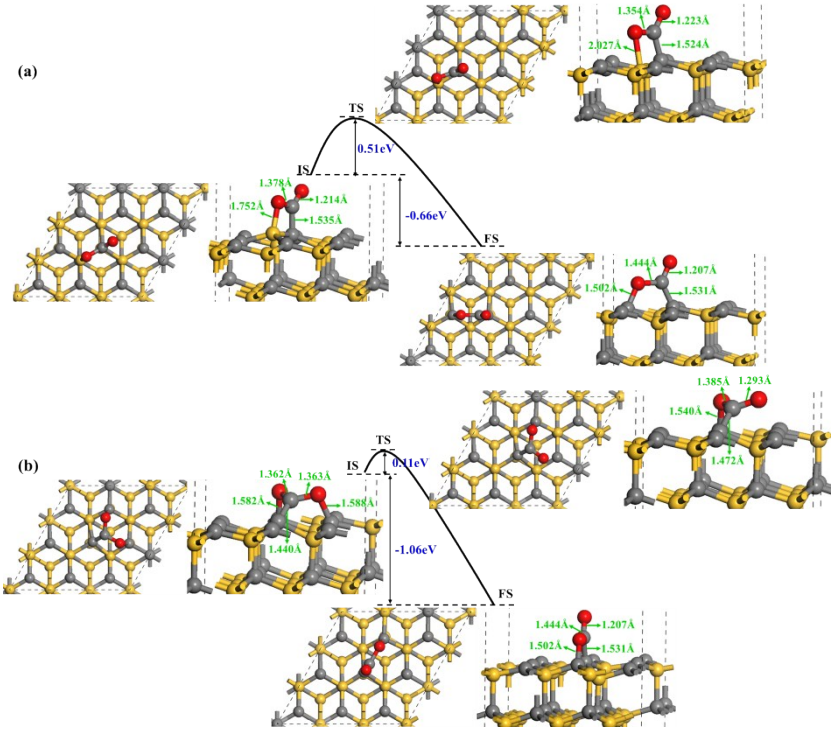

Fig. S6 (a) The minimum energy path for transformation from the adsorption configuration in Fig. 4(a) to that in Fig. 4(d); (b) The minimum energy path for transformation from the adsorption configuration in Fig. 4(b) to that in Fig. 4(d). Gary, red and yellow balls represent C, O, and Si atoms, respectively.

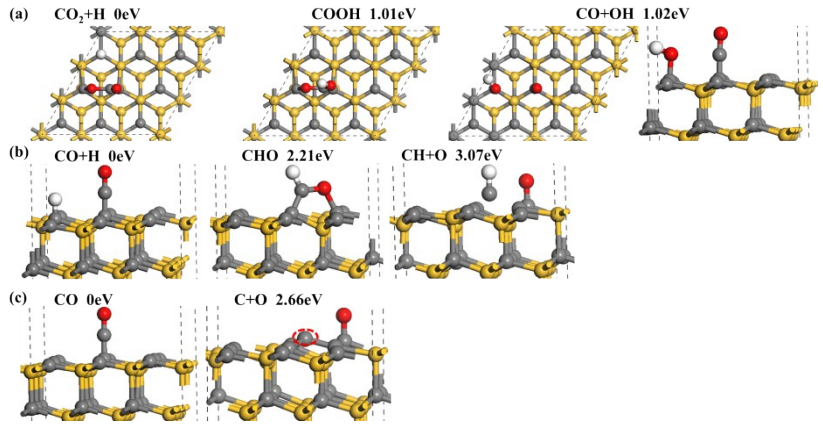

Fig. S7 (a) Optimized structures of CO_2+H co-adsorption, COOH group, and CO+OH co-adsorption on Sic (000) surface, the energies are relative to CO_2+H co-adsorption state. There is no HCOO adsorption structure because after fully optimization the HCOO group turns into CO_2+H co-adsorption state; (b) Optimized structures of CO+H co-adsorption, CHO group, and CH+O co-adsorption on SiC (000) surface, the energies are relative to CO+H co-adsorption state; (c) Optimized structures of CO and C+O co-adsorption on Sic (000) surface, the energies are relative CO adsorption states. Gary, red, yellow and white balls represent C, O, Si and H atoms, respectively.