A DFT Insight into the Tuning Effect of Potassium Promoter on

the Formation of Carbon Atoms via carburization gases

dissociation on Iron-Based Catalysts

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Figure S1. The energy profiles of C_2H_4 dissociation on Fe(110), as well as the top and side view of the configurations for the corresponding intermediates. The Fe, O, C and H atoms are given in grayish blue, red, black and white, respectively.



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Figure S9. The top and side view structures of 2CH+H, C+CH+3H and 2C+4H on Fe(110). The Fe, C and H atoms are given in grayish blue, black and white, respectively.

| Fe(110) | | | | Fe(110)-K ₂ O | | | |
|---|---|--|--|---|--|--|---|
| element steps | d_{CH} | <i>d</i> _{CC} | <i>d</i> _{C0} | element steps | <i>d</i> _{CH} | <i>d</i> _{CC} | <i>d</i> _{C0} |
| | (Å) | (Å) | (Å) | | (Å) | (Å) | (Å) |
| $C_2H_4 \rightarrow C_2H_3 + H$ | 1.585 | / | / | $C_2H_4 \rightarrow C_2H_3 + H$ | 1.584 | / | / |
| $C_2H_3+H\rightarrow CHCH+2H$ | 1.344 | / | / | $C_2H_3+H\rightarrow CHCH+2H$ | 1.463 | / | / |
| $\rm CHCH+2H{\rightarrow}2\rm CH+2H$ | / | 2.027 | / | $\text{CHCH+2H} {\rightarrow} \text{CCH+3H}$ | 1.544 | / | / |
| $2CH+2H\rightarrow C+CH+3H$ | 1.418 | / | / | CCH+2H→C+CH+3H | 1.461 | / | / |
| $C+CH+3H\rightarrow 2C+4H$ | 1.489 | / | / | $C+CH+3H\rightarrow 2C+4H$ | / | 1.908 | / |
| СО+2Н→СНО+Н | 1.536 | / | / | СО+2Н→СНО+Н | 1.231 | / | / |
| СНО+Н→СН+О+Н | / | / | 1.739 | СНО+Н→СН+О+Н | / | / | 1.844 |
| CH+O+H→C+O+2H | 1.410 | / | / | $CH+O+H\rightarrow C+O+2H$ | 1.435 | / | / |
| Fe(211) | | | | | | | |
| Fe(2 | 211) | | | Fe(211) |)-K ₂ O | | |
| Fe(2 | 211) d _{Сн} | <i>d</i> _{CC} | <i>d</i> _{C0} | Fe(211 |) -К₂О <i>d</i> _{СН} | d _{CC} | <i>d</i> _{C0} |
| Fe(2 element steps | 211) d _{Сн} (Å) | d _{CC} (Å) | d _{C0} (Å) | Fe(211) element steps |) -К₂О <i>d</i> _{С…Н} (Å) | d _{CC} (Å) | d _{C0} (Å) |
| Fe(2 element steps C2H4→C2H3+H | 211) <i>d</i> _{CH} (Å) 1.585 | d _{CC} (Å) | d _{C0} (Å) | Fe(211) element steps $C_2H_4 \rightarrow C_2H_3 + H$ |)- К₂О <i>d</i> _{С…Н} (Å) 1.555 | d _{CC} (Å) | d _{C0} (Å) ∕ |
| Fe(2element steps $C_2H_4 \rightarrow C_2H_3 + H$ $C_2H_3 + H \rightarrow CCH_2 + 2H$ | 211) <i>d</i> _{CH} (Å) 1.585 1.497 | d _{CC} (Å) / | d _{C0} (Å) / | Fe(211element steps $C_2H_4 \rightarrow C_2H_3 + H$ $C_2H_3 + H \rightarrow CHCH + 2H$ |)- K₂O <i>d</i> _{CH} (Å) 1.555 1.539 | d _{CC} (Å) / | d _{C0} (Å) / |
| Fe(2 element steps $C_2H_4 \rightarrow C_2H_3+H$ $C_2H_3+H \rightarrow CCH_2+2H$ $CCH_2+2H \rightarrow CCH+3H$ | 211) <i>d</i> _{CH} (Å) 1.585 1.497 1.572 | d _{CC} (Å) / / | d _{C0} (Å) / / | Fe(211element steps $C_2H_4 \rightarrow C_2H_3 + H$ $C_2H_3 + H \rightarrow CHCH + 2H$ $CHCH + 2H \rightarrow CCH + 3H$ |)-К₂О <i>d</i> _{Сн} (Å) 1.555 1.539 1.501 | d _{cc} (Å) / / | d _{C0} (Å) / / |
| Fe(2element steps $C_2H_4 \rightarrow C_2H_3 + H$ $C_2H_3 + H \rightarrow CCH_2 + 2H$ $CCH_2 + 2H \rightarrow CCH + 3H$ $CCH_2 + 3H \rightarrow CC + 4H$ | 211) d _{CH} (Å) 1.585 1.497 1.572 1.571 | d _C c (Å) / / | d _{C0} (Å) / / | Fe(211element steps $C_2H_4 \rightarrow C_2H_3 + H$ $C_2H_3 + H \rightarrow CHCH + 2H$ $CHCH + 2H \rightarrow CCH + 3H$ $CCH + 3H \rightarrow CC + 4H$ |)-К ₂ О dcн (Å) 1.555 1.539 1.501 1.461 | dcc (Å) / / | d _{C0} (Å) / / |
| Fe(2element steps $C_2H_4 \rightarrow C_2H_3 + H$ $C_2H_3 + H \rightarrow CCH_2 + 2H$ $CCH_2 + 2H \rightarrow CCH + 3H$ $CCH_2 + 2H \rightarrow CCH + 3H$ $CCH + 3H \rightarrow CC + 4H$ $CC + 4H \rightarrow 2C + 4H$ | 211) d _{CH} (Å) 1.585 1.497 1.572 1.571 / | d _C c (Å) / / / 1.939 | d _{co} (Å) / / / | Fe(211element steps $C_2H_4 \rightarrow C_2H_3 + H$ $C_2H_3 + H \rightarrow CHCH + 2H$ $CHCH + 2H \rightarrow CCH + 3H$ $CCH + 3H \rightarrow CC + 4H$ $CC + 4H \rightarrow 2C + 4H$ |)-К ₂ О d _{Cн} (Å) 1.555 1.539 1.501 1.461 | dcc (Å) / / / 2.009 | d _{C0} (Å) / / / |
| Fe(2element steps $C_2H_4 \rightarrow C_2H_3 + H$ $C_2H_3 + H \rightarrow CCH_2 + 2H$ $CCH_2 + 2H \rightarrow CCH + 3H$ $CCH_3H \rightarrow CC+4H$ $CC+4H \rightarrow 2C+4H$ $CC+2H \rightarrow CHO+H$ | 211) d _{CH} (Å) 1.585 1.497 1.572 1.571 / / | dcc (Å) / / / 1.939 / | dco (Å) / / / / | Fe(211element steps $C_2H_4 \rightarrow C_2H_3 + H$ $C_2H_3 + H \rightarrow CHCH + 2H$ $CHCH + 2H \rightarrow CCH + 3H$ $CCH + 3H \rightarrow CC + 4H$ $CC + 4H \rightarrow 2C + 4H$ |)-К ₂ О <i>d</i> _{Сн} (Å) 1.555 1.539 1.501 1.461 / | d _{cc} (Å) / / / 2.009 | dco (Å) / / / |
| Fe(2element steps $C_2H_4 \rightarrow C_2H_3 + H$ $C_2H_3 + H \rightarrow CCH_2 + 2H$ $CCH_2 + 2H \rightarrow CCH + 3H$ $CCH_2 + 2H \rightarrow CCH + 3H$ $CCH + 3H \rightarrow CC + 4H$ $CC + 4H \rightarrow 2C + 4H$ $CO + 2H \rightarrow CHO + H$ $CHO + H \rightarrow CH + O + H$ | 211) d _{CH} (Å) 1.585 1.497 1.572 1.571 / / / | d _C c (Å) / / / 1.939 / | d _{C0} (Å) / / / / / 1.819 | Fe(211element steps $C_2H_4 \rightarrow C_2H_3 + H$ $C_2H_3 + H \rightarrow CHCH + 2H$ $CHCH + 2H \rightarrow CCH + 3H$ $CCH + 3H \rightarrow CC + 4H$ $CC + 4H \rightarrow 2C + 4H$ $CO + 2H \rightarrow C + O + 2H$ |)-К ₂ О d _{Сн} (Å) 1.555 1.539 1.501 1.461 / | dcc (Å) / / / 2.009 | d _{C0} (Å) / / / / 1.887 |

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