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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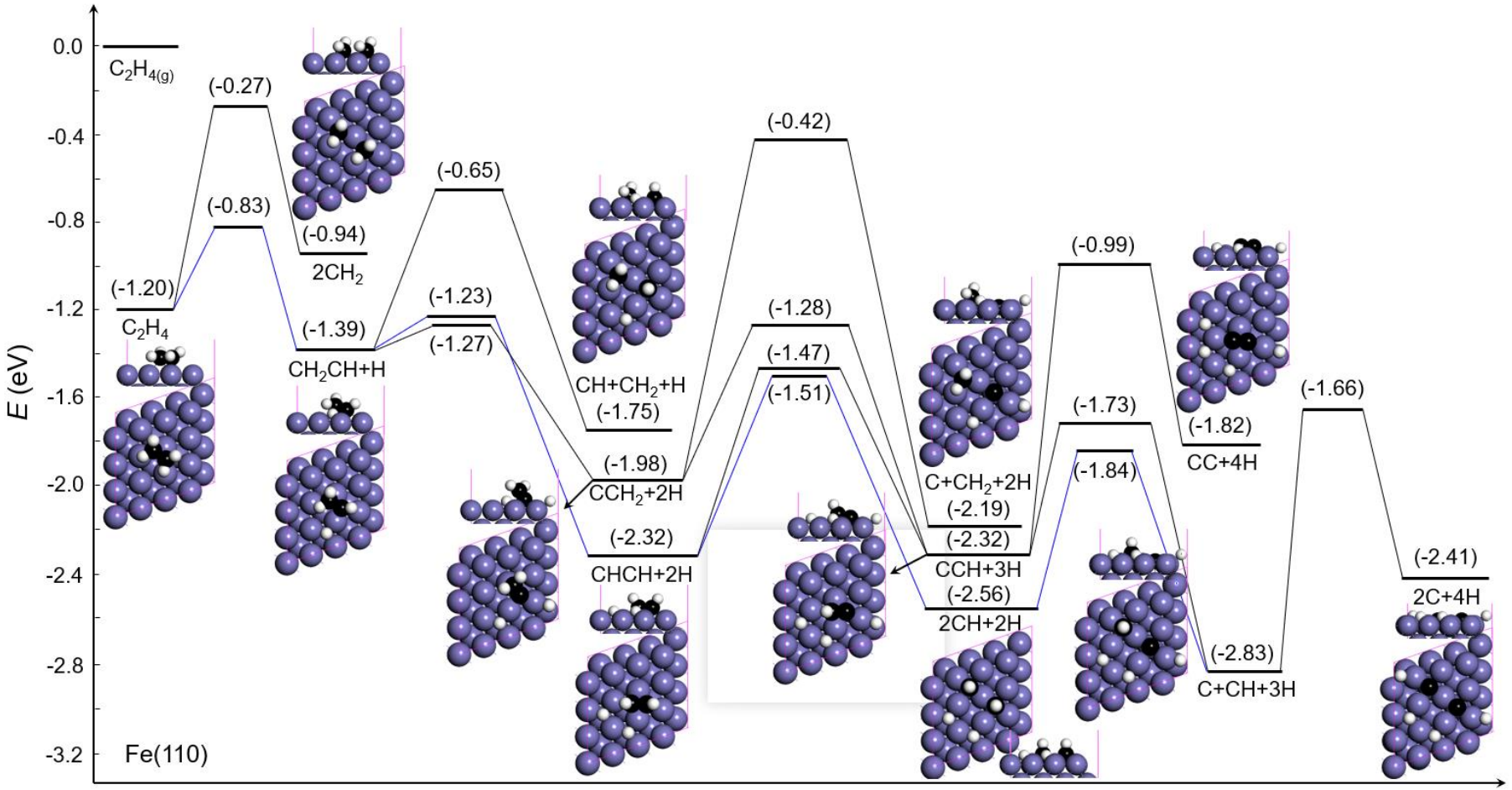

Figure S1. The energy profiles of C_2H_4 dissociation on Fe(110), as well as the top and side view of the configurations for the corresponding intermediates. The Fe, O, C and H atoms are given in grayish blue, red, black and white, respectively.

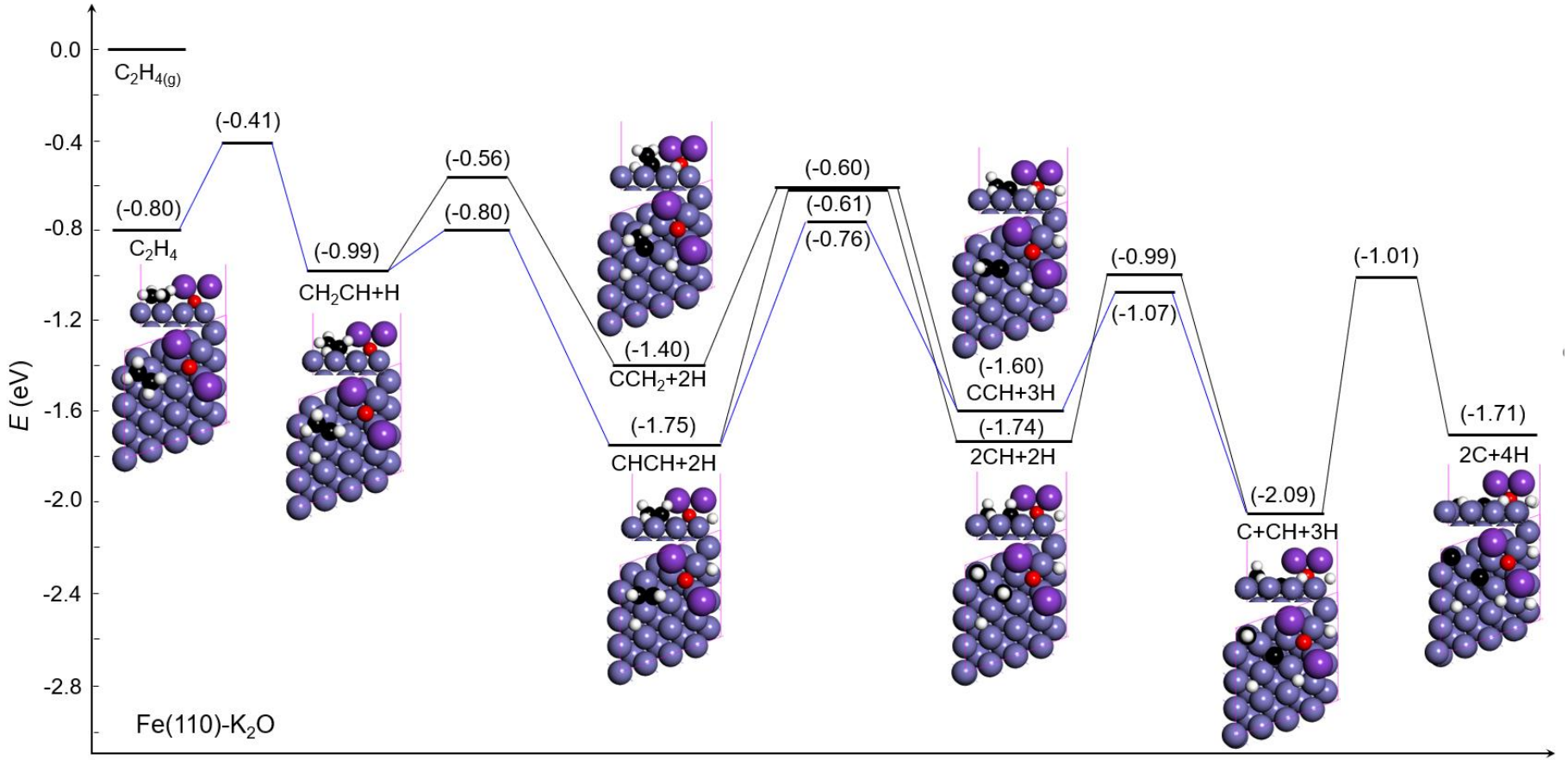

Figure S2. The energy profiles of C_2H_4 dissociation on Fe(110)-K_2O, as well as the top and side view of the configurations for the corresponding intermediates. The Fe, K, O, C and H atoms are given in grayish blue, purple, red, black and white, respectively.

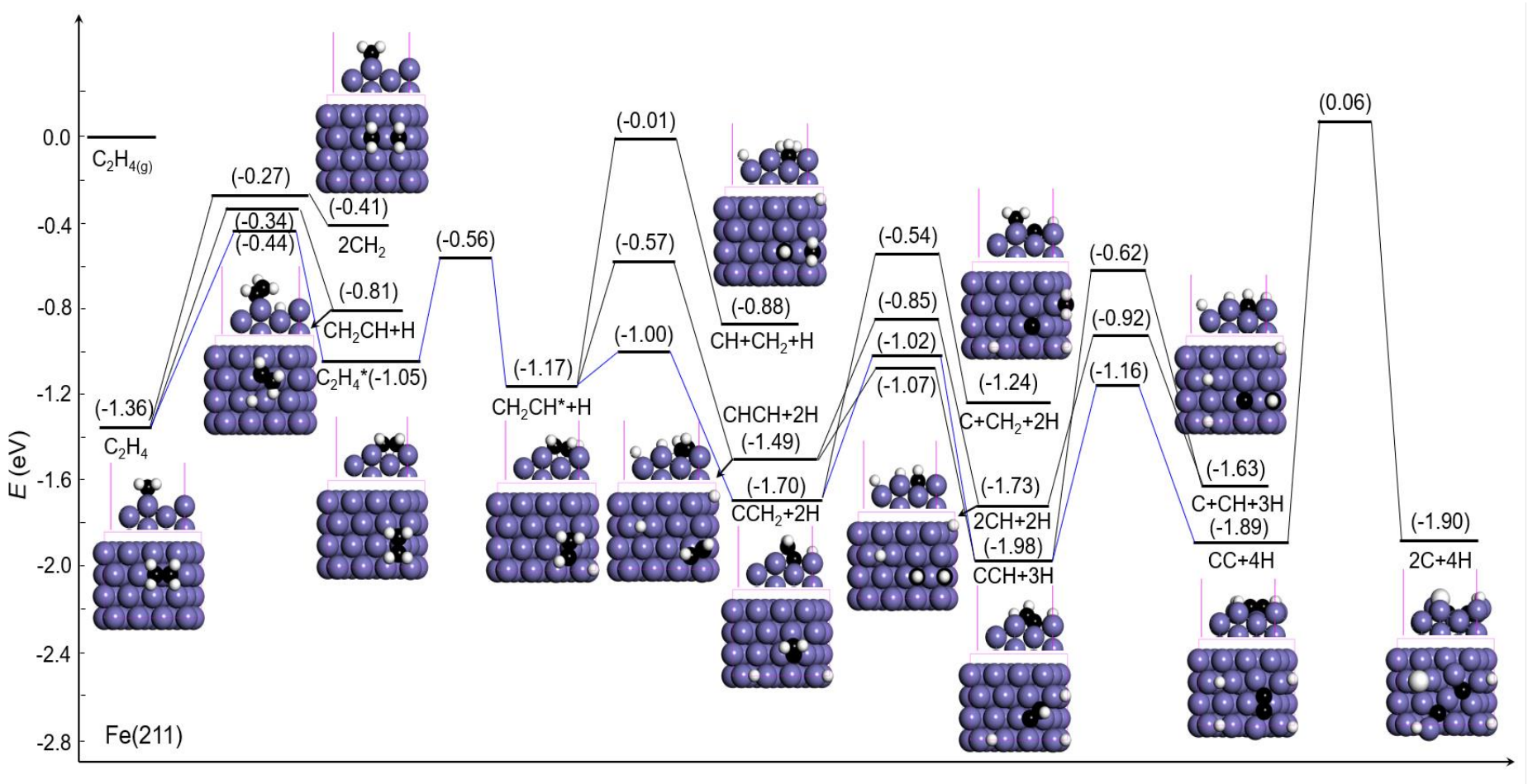

Figure S3. The energy profiles of C_2H_4 dissociation on Fe(211), as well as the top and side view of the configurations for the corresponding intermediates. The Fe, O, C and H atoms are given in grayish blue, red, black and white, respectively.

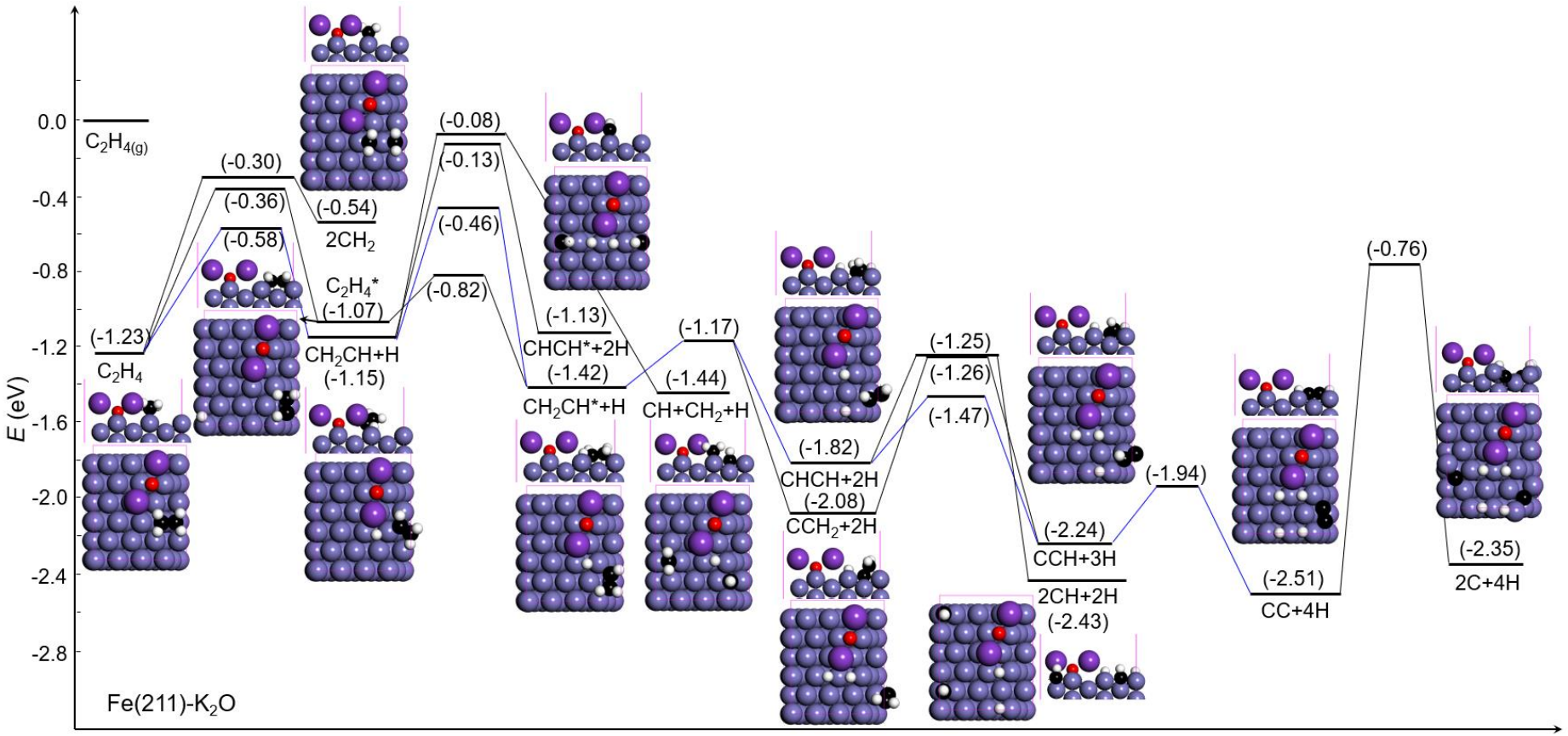

Figure S4. The energy profiles of C_2H_4 dissociation on Fe(211)-K_2O, as well as the top and side view of the configurations for the corresponding intermediates. The Fe, K, O, C and H atoms are given in grayish blue, purple, red, black and white, respectively.

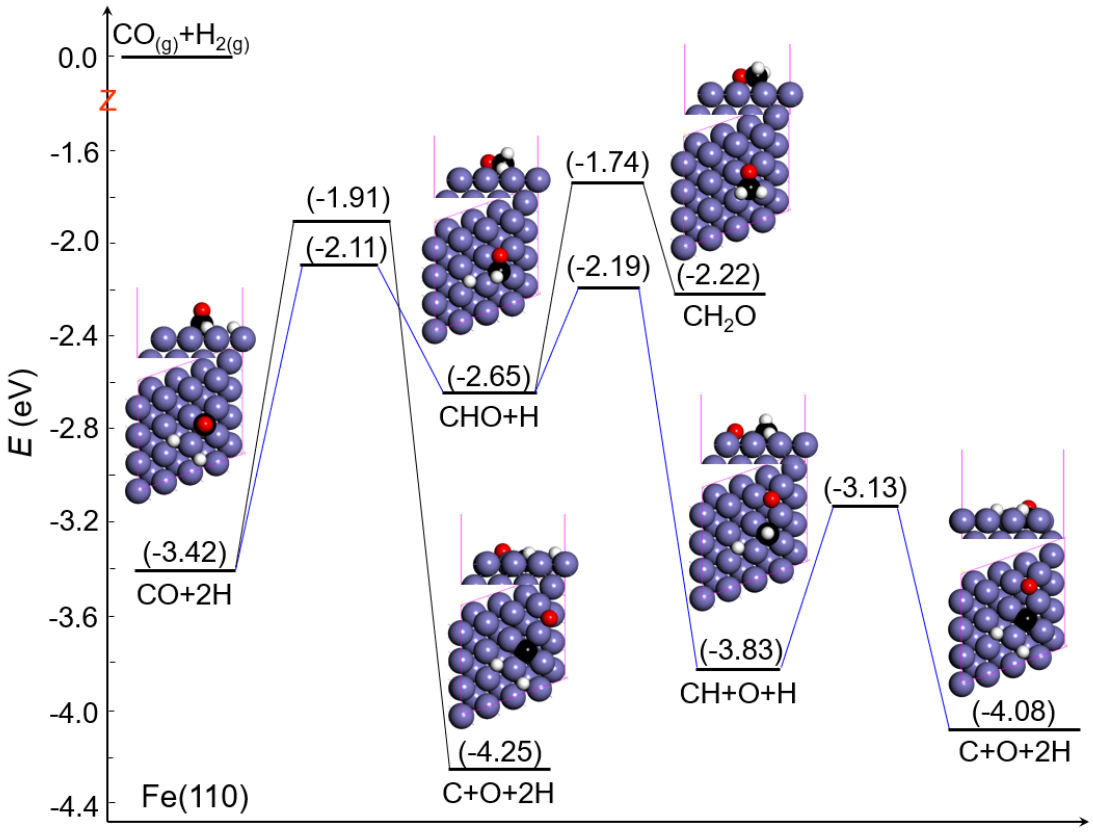

Figure S5. The energy profiles of CO/H_2 dissociation on Fe(110), as well as the top and side view of the configurations for the corresponding intermediates. The Fe, O, C and H atoms are given in grayish blue, red, black and white, respectively.

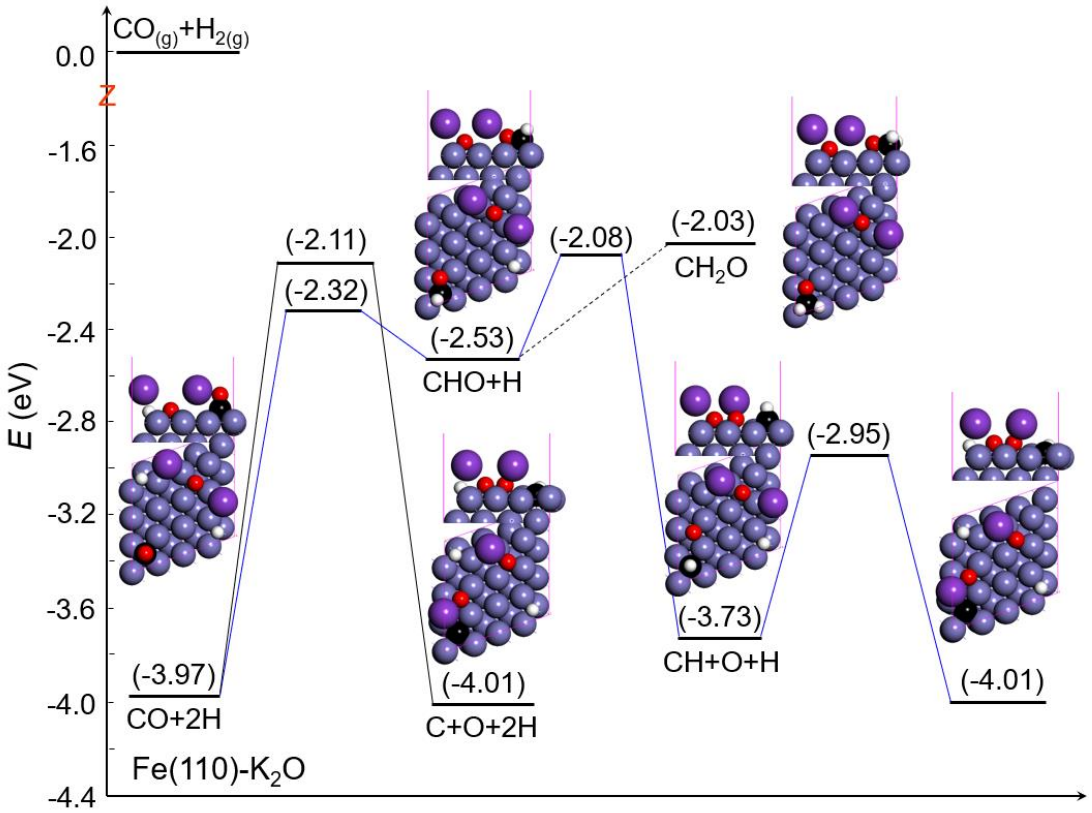

Figure S6. The energy profiles of CO/H_2 dissociation on Fe(110)-K_2O, as well as the top and side view of the configurations for the corresponding intermediates. The Fe, K, O, C and H atoms are given in grayish blue, purple, red, black and white, respectively.

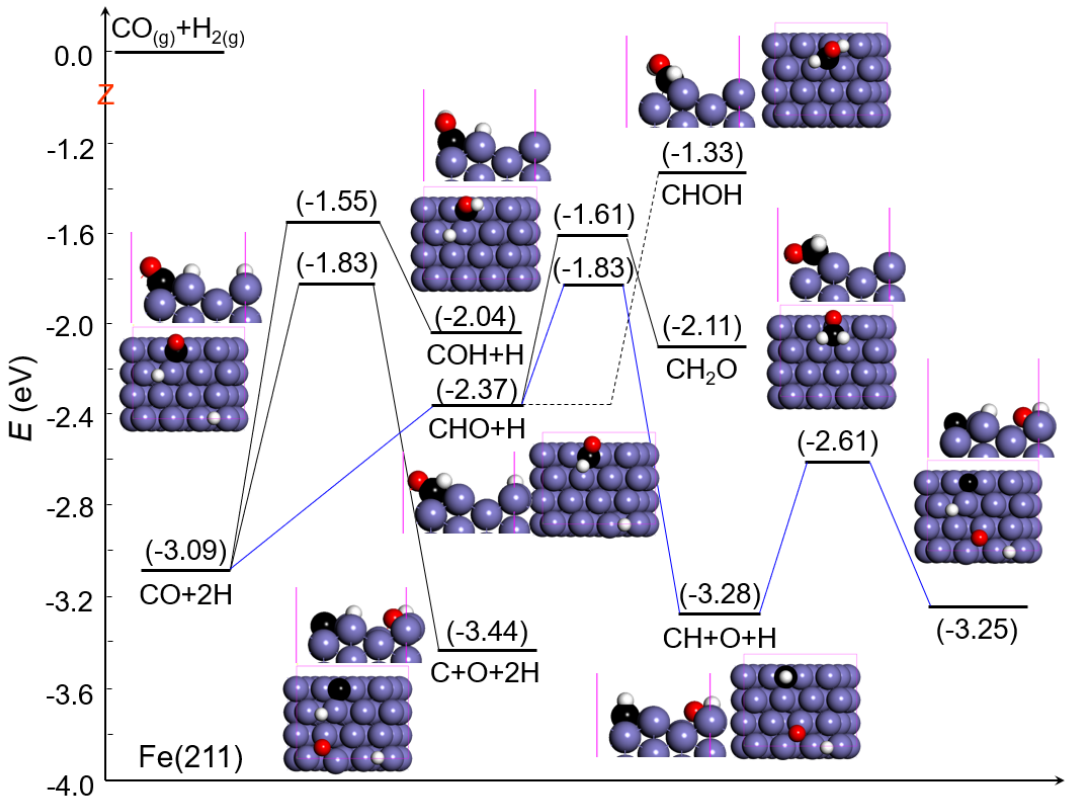

Figure S7. The energy profiles of CO/H_2 dissociation on Fe(211), as well as the top and side view of the configurations for the corresponding intermediates. The Fe, O, C and H atoms are given in grayish blue, red, black and white, respectively.

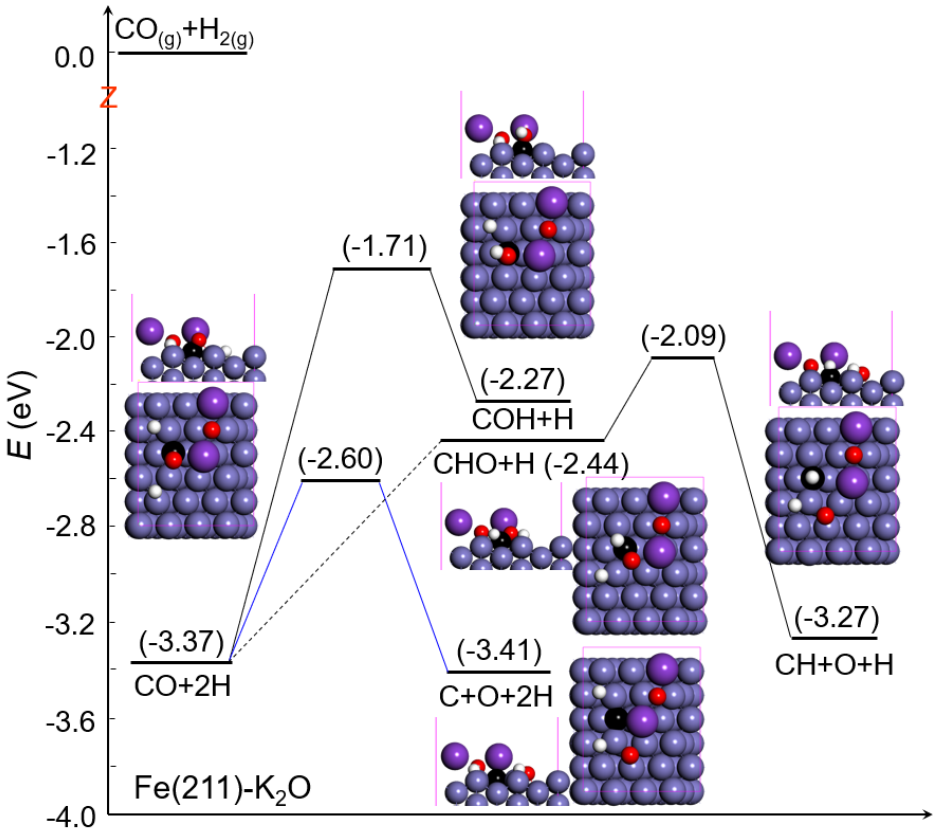

Figure S8. The energy profiles of CO/H_2 dissociation on Fe(211)-K_2O, as well as the top and side view of the configurations for the corresponding intermediates. The Fe, K, O, C and H atoms are given in grayish blue, purple, red, black and white, respectively.

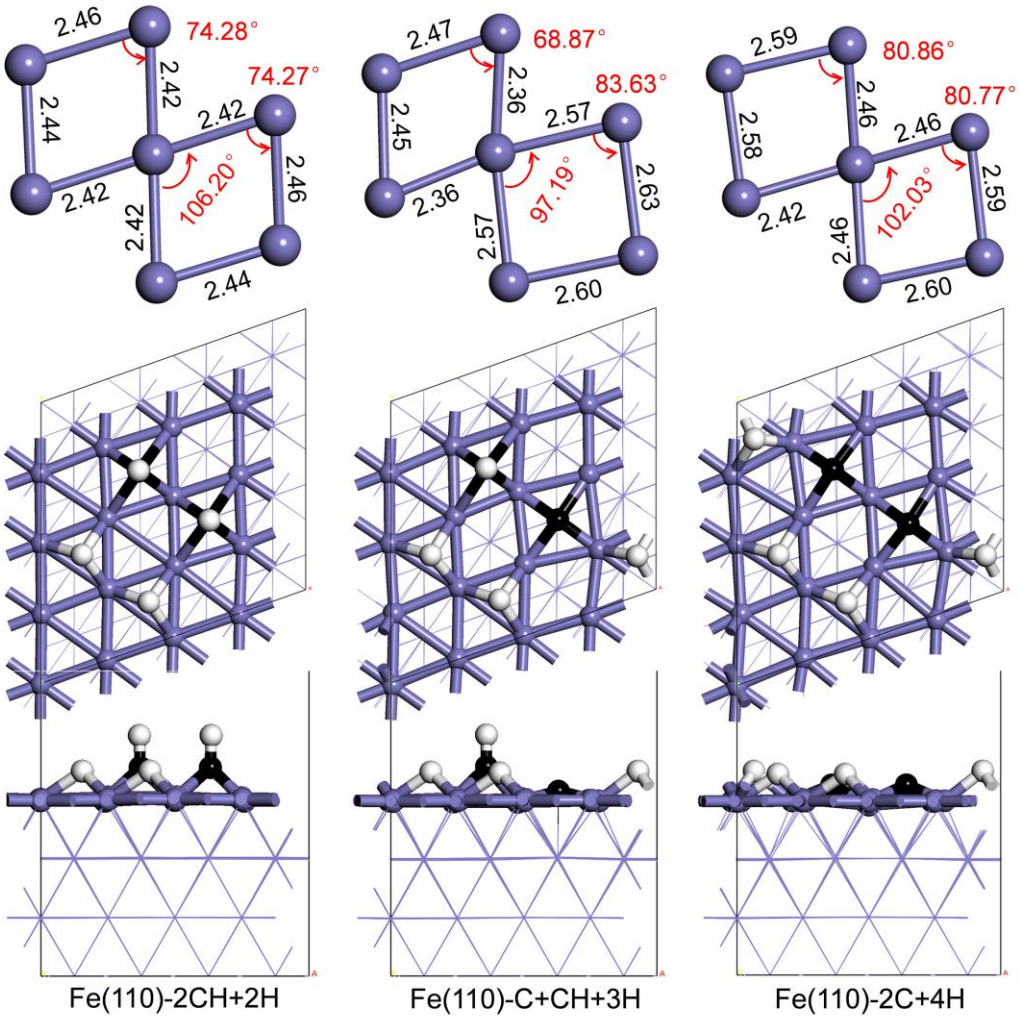

Figure S9. The top and side view structures of 2CH+H, C+CH+3H and 2C+4H on Fe(110). The Fe, C and H atoms are given in grayish blue, black and white, respectively.

Table S1. The distances between the two atoms (d, Å) be dissociated in the transition states of the element steps for C_2H_4 and CO/H_2 dissociation on Fe(110), Fe(110)-K_2O, Fe(211) and Fe(211)-K_2O surfaces

Fe(110)				**Fe(110)-K_2O**			
element steps	$d_{C...H}$ (Å)	$d_{C...C}$ (Å)	$d_{C...O}$ (Å)	element steps	$d_{C...H}$ (Å)	$d_{C...C}$ (Å)	$d_{C...O}$ (Å)
C_2H_4→C_2H_3+H	1.585	/	/	C_2H_4→C_2H_3+H	1.584	/	/
C_2H_3+H→CHCH+2H	1.344	/	/	C_2H_3+H→CHCH+2H	1.463	/	/
CHCH+2H→2CH+2H	/	2.027	/	CHCH+2H→CCH+3H	1.544	/	/
2CH+2H→C+CH+3H	1.418	/	/	CCH+2H→C+CH+3H	1.461	/	/
C+CH+3H→2C+4H	1.489	/	/	C+CH+3H→2C+4H	/	1.908	/
CO+2H→CHO+H	1.536	/	/	CO+2H→CHO+H	1.231	/	/
CHO+H→CH+O+H	/	/	1.739	CHO+H→CH+O+H	/	/	1.844
CH+O+H→C+O+2H	1.410	/	/	CH+O+H→C+O+2H	1.435	/	/
Fe(211)				**Fe(211)-K_2O**			
element steps	$d_{C...H}$ (Å)	$d_{C...C}$ (Å)	$d_{C...O}$ (Å)	element steps	$d_{C...H}$ (Å)	$d_{C...C}$ (Å)	$d_{C...O}$ (Å)
C_2H_4→C_2H_3+H	1.585	/	/	C_2H_4→C_2H_3+H	1.555	/	/
C_2H_3+H→CCH_2+2H	1.497	/	/	C_2H_3+H→CHCH+2H	1.539	/	/
CCH_2+2H→CCH+3H	1.572	/	/	CHCH+2H→CCH+3H	1.501	/	/
CCH+3H→CC+4H	1.571	/	/	CCH+3H→CC+4H	1.461	/	/
CC+4H→2C+4H	/	1.939	/	CC+4H→2C+4H	/	2.009	/
CO+2H→CHO+H	/	/	/	CO+2H→C+O+2H	/	/	1.887
CHO+H→CH+O+H	/	/	1.819				
CH+O+H→C+O+2H	1.482	/	/				