An investigation on the conversion of ethylene to ethylidyne on Pt(100) and Pd(100) using density functional theory

SUPPORTING INFORMATION

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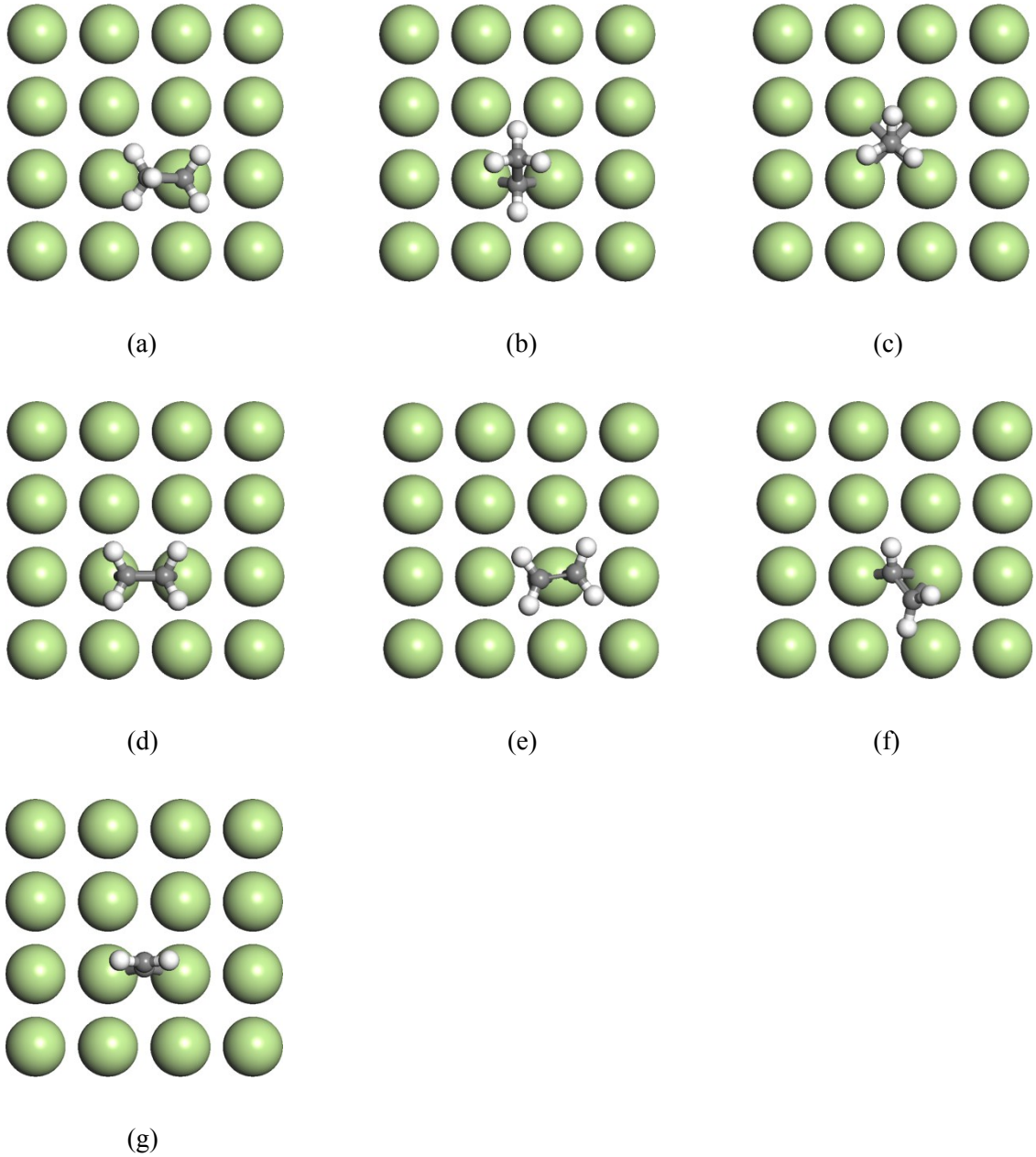


Figure S1. The adsorption of intermediates on Pd(100). (a) CH_3CH_2; (b) CH_3CH; (c) CH_3C; (d) CH_2CH_2 in di-σ mode; (e) CH_2CH_2 in π mode; (f) CH_2CH; (g) CH_2C. Carbon atoms are gray, hydrogen atoms white, and palladium atoms green.

In order to present adsorption configurations clearly, here we only show the top layer of Pd(100) and adsorbates.

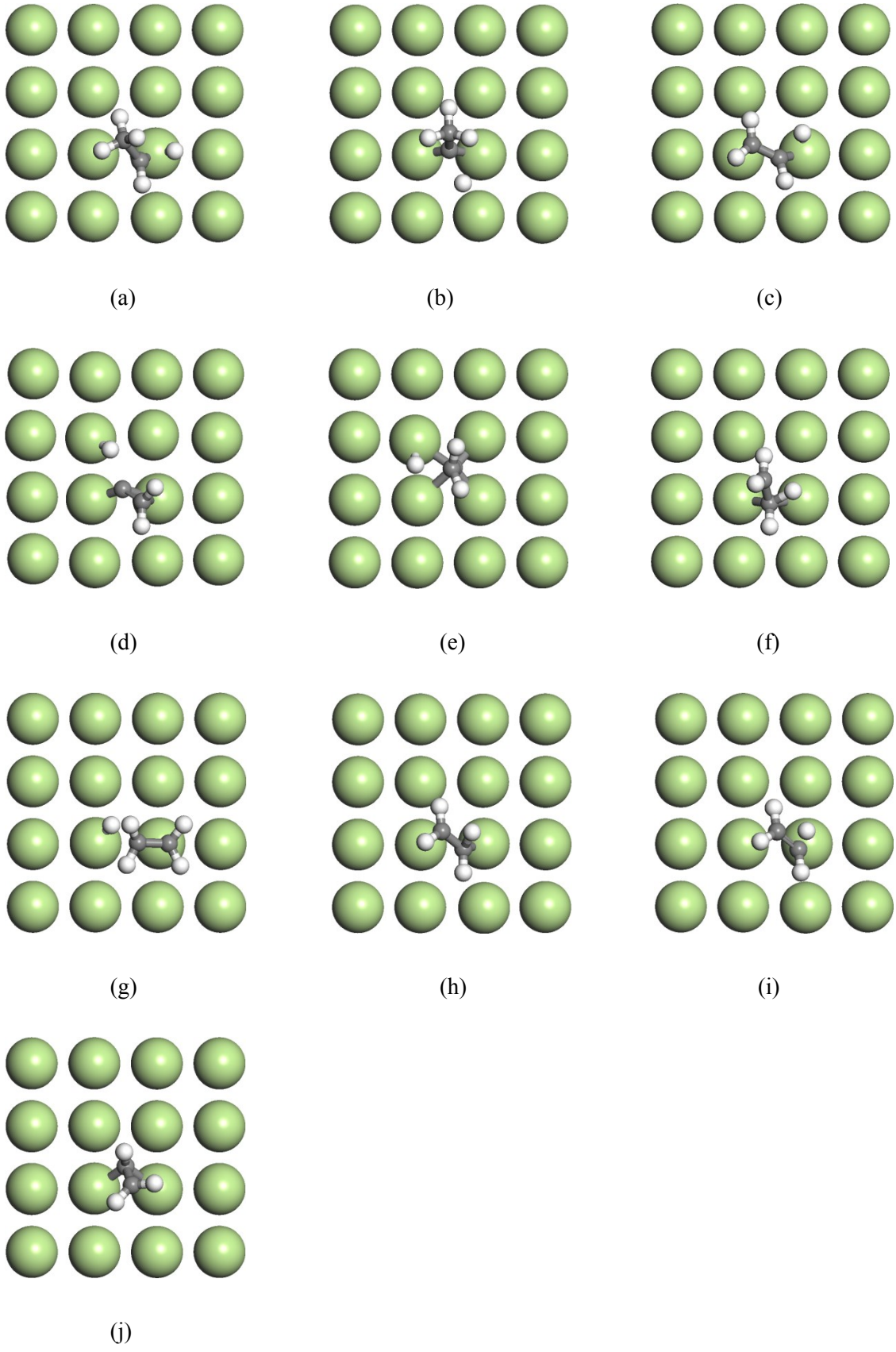
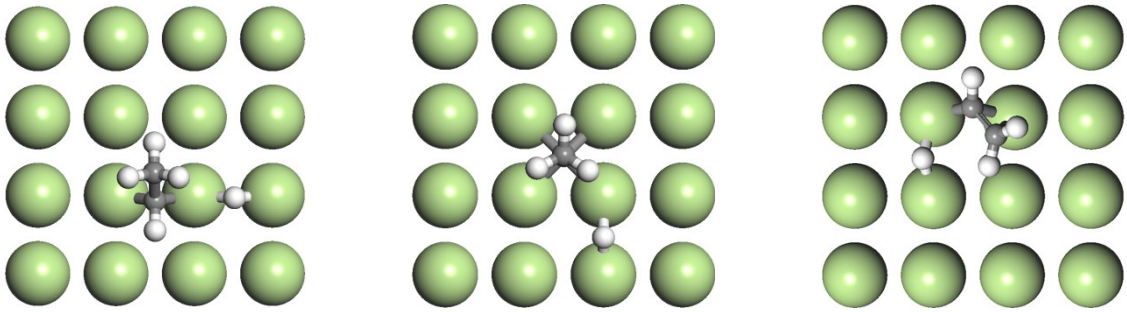
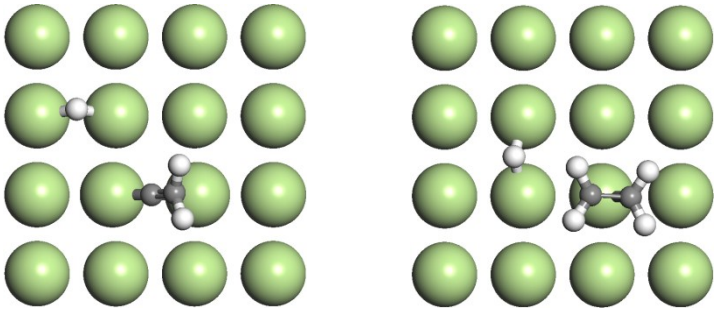


Figure S2. Geometric structures of the transition state (TS) of intermediate reactions on Pd(100). (a) $CH_3CH_2 \rightarrow CH_3CH+H$; (b) $CH_3CH \rightarrow CH_3C+H$; (c) $CH_2CH2(\sigma) \rightarrow CH_2CH+H$; (d) $CH_2CH \rightarrow CH_2C+H$; (e) $CH_2C+H \rightarrow CH_3C$; (f) $CH_2CH+H \rightarrow CH_3CH$; (g) $CH_2CH_2(\pi)+H \rightarrow CH_3CH_2$; (h) $CH_2CH_2(\sigma) \rightarrow CH_3CH$; (i) $CH_2CH_2(\pi) \rightarrow CH_3CH$; (j) $CH_2CH \rightarrow CH_3C$. Carbon atoms are gray, hydrogen atoms white, and palladium atoms green.

In order to present adsorption configurations clearly, here we only show the top layer of Pd(100) and adsorbates.



(a) (b) (c)



(d) (e)

Figure S3 Coadsorption of intermediates and H on Pd(100). (a) ethylidene+H; (b) ethylidyne+H; (c) vinyl+H; (d) vinylidene+H; (e) ethylene(π)+H

In order to present adsorption configurations clearly, here we only show the top layer of Pd(100) and adsorbates.

Table S1: Optimized structural parameters(Å) for the Initial State(IS), Transition State(TS), and Final State(FS) of elementary reactions in the formation network of ethylidyne on Pt(100)

	Parameter	IS	TS	FS
$CH_3CH_2 \rightarrow CH_3CH+H$	C-C	1.51	1.46	1.50
	C-H[a]	1.10	1.64	2.97
	C-Pt[b]	2.07	1.97	2.04,2.06
	H-Pt[c]	-	1.73	1.73,1.76
$CH_3CH \rightarrow CH_3C+H$	C-C	1.50	1.45	1.50
	C-H	1.10	1.55	3.23
	C-Pt	2.04,2.05	1.94,1.96	2.12,2.17,2.20,2.20
	H-Pt	-	1.77	1.71,1.78
$CH_2CH_2 \rightarrow CH_2CH+H$	C-C	1.48	1.41	1.42
	C-H[a]	1.10	1.53	2.56
	C-Pt[b]	2.09;2.09	1.98;2.15	2.01,2.15;2.18
	H-Pt	-	1.68	1.70,1.78
$CH_2CH \rightarrow CH_2C+H$	C-C	1.42	1.39	1.39
	C-H	1.09	2.42	3.91
	C-Pt	1.99,2.17;2.19	1.84,2.00;2.21	1.86,2.02;2.22
	H-Pt	-	1.58	1.73,1.75
$CH_2C+H \rightarrow CH_3C$	C-C	1.39	1.42	1.50
	C-H	4.81	1.74	1.10
	C-Pt	1.86,2.02;2.22	2.10,2.13,2.14	2.15,2.16,2.17,2.19
	H-Pt	1.73,1.75	1.71	-
$CH_2CH+H \rightarrow CH_3CH$	C-C	1.42	1.45	1.50
	C-H	2.94	2.00	1.10
	C-Pt	2.01,2.16;2.19	2.02,2.07	2.04,2.05
	H-Pt	1.70,1.78	2.58,2.89	-
$CH_2CH_2+H \rightarrow CH_3CH_2$	C-C	1.42	1.43	1.51
	C-H	3.06	1.76	1.10
	C-Pt	2.17,2.17	2.17	2.07
	H-Pt	1.72,1.76	1.60	-
$CH_2CH_2(\sigma) \rightarrow CH_3CH$	C-C	1.48	1.43	1.50
	C-H	1.10	1.32	1.10
	C-Pt	2.09;2.09	1.97	2.04,2.05
$CH_2CH_2(\pi) \rightarrow CH_3CH$	C-C	1.42	1.39	1.50
	C-H	1.09	1.31	1.10
	C-Pt	2.17,2.17	1.96	2.04,2.05
$CH_2CH \rightarrow CH_3C$	C-C	1.42	1.44	1.50
	C-H	1.10	1.44	1.10
	C-Pt	1.99,2.17;2.19	1.99,2.05	2.15,2.16,2.17,2.19

[a] Distance that characterizes the bond that is breaking /forming during the reaction.
[b] The values before the semicolon refer to the distance of the Pt atom and the C atom bound to more surface atoms
[c] The distance of dissociating H atom and the surface atom.

Table S2: Optimized structural parameters(Å) for the Initial State(IS), Transition State(TS), and Final State(FS) of elementary reactions in the formation network of ethylidyne on Pd(100)

	Parameter	IS	TS	FS
$CH_3CH_2 \rightarrow CH_3CH+H$	C-C	1.51	1.50	1.50
	C-H[a]	1.10	1.62	2.83
	C-Pd[b]	2.05	1.93	2.01,2.02
	H-Pd[c]	-	1.68	1.73,1.78
$CH_3CH \rightarrow CH_3C+H$	C-C	1.50	1.49	1.51
	C-H	1.11	1.61	3.16
	C-Pd	2.01,2.01	1.95,1.95	2.13,2.14,2.14,2.14
	H-Pd	-	1.88	1.67,1.81
$CH_2CH_2 \rightarrow CH_2CH+H$	C-C	1.44	1.40	1.40
	C-H	1.10	1.54	2.56
	C-Pd	2.14;2.14	2.18;2.05	2.14,2.00;2.24
	H-Pd	-	1.65	1.70;1.77,
$CH_2CH \rightarrow CH_2C+H$	C-C	1.39	1.38	1.36
	C-H	1.10	1.91	3.98
	C-Pd	2.01,2.13;2.33	1.95,2.07;2.30	1.87;1.98
	H-Pd	-	1.79	1.74,1.74
$CH_2C+H \rightarrow CH_3C$	C-C	1.36	1.43	1.50
	C-H	4.69	1.67	1.10
	C-Pd	1.87,1.98	2.01,2.03,2.12,2.33	2.14,2.14,2.14,2.14
	H-Pd	1.74,1.74	1.75	-
$CH_2CH+H \rightarrow CH_3CH$	C-C	1.40	1.43	1.50
	C-H	2.92	1.26	1.10
	C-Pd	2.00,2.14;2.24	2.12,2.13	2.01,2.01
	H-Pd	1.70,1.77	2.09	-
$CH_2CH_2+H \rightarrow CH_3CH_2$	C-C	1.40	1.41	1.51
	C-H	3.29	1.77	1.10
	C-Pd	2.15;2.21	2.12	2.05
	H-Pd	1.70;1.72	1.66	-
$CH_2CH_2(\sigma) \rightarrow CH_3CH$	C-C	1.44	1.43	1.50
	C-H	1.10	1.30	1.10
	C-Pd	2.14;2.14	1.99	2.01,2.01
$CH_2CH_2(\pi) \rightarrow CH_3CH$	C-C	1.40	1.41	1.50
	C-H	1.09	1.31	1.10
	C-Pd	2.23;2.23	1.97	2.01,2.01
$CH_2CH \rightarrow CH_3C$	C-C	1.39	1.44	1.50
	C-H	1.10	1.24	1.10
	C-Pd	2.01,2.13;2.33	2.10,2.12	2.14,2.14,2.14,2.14

[a] Distance that characterizes the bond that is breaking /forming during the reaction.
[b] The values before the semicolon refer to the distance of the Pd atom and the C atom bound to more surface atoms
[c] The distance of dissociating H atom and the surface atom.