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) CH₃CH₂; (b) CH₃CH; (c) CH₃C; (d) CH₂CH₂ in di-σ mode; (e) CH₂CH₂ in π mode; (f) CH₂CH; (g) CH₂C. 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$_3$CH$_2$→CH$_3$CH+H; (b) CH$_3$CH→CH$_3$C+H; (c) CH$_2$CH$_2$(σ)→CH$_2$CH+H; (d) CH$_3$CH→CH$_2$C+H; (e) CH$_2$C+H→CH$_3$C; (f) CH$_2$CH+H→CH$_3$CH; (g) CH$_2$CH$_2$(π)+H→CH$_3$CH$_2$; (h) CH$_2$CH$_2$(σ)→CH$_3$CH; (i) CH$_2$CH$_2$(π)→CH$_3$CH; (j) CH$_2$C→CH$_3$C. 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 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)

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<th>IS</th>
<th>TS</th>
<th>FS</th>
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<td>1.46</td>
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<td>1.97</td>
<td>2.04, 2.06</td>
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<tr>
<td>H-Pt&lt;sup&gt;c&lt;/sup&gt;</td>
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<td>1.73</td>
<td>1.73, 1.76</td>
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<td>C-Pt</td>
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<td>1.71, 1.78</td>
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<td>1.70, 1.78</td>
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<td>1.73, 1.75</td>
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<td>H-Pt</td>
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<td>1.45</td>
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<td>2.02, 2.07</td>
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<sup>a</sup> Distance that characterizes the bond that is breaking/forming during the reaction.

<sup>b</sup> The values before the semicolon refer to the distance of the Pt atom and the C atom bound to more surface atoms.

<sup>c</sup> The distance of dissociating H atom and the surface atom.
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<td>C-Pd</td>
<td>2.01,2.13;2.33</td>
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\textsuperscript{a} Distance that characterizes the bond that is breaking/forming during the reaction.
\textsuperscript{b} The values before the semicolon refer to the distance of the Pd atom and the C atom bound to more surface atoms.
\textsuperscript{c} The distance of dissociating H atom and the surface atom.