We present kinetic Monte Carlo simulations of ethylene conversion to ethylidyne on Pd(1 1 1) and Pt(1 1 1) surfaces, on the basis of reaction enthalpies and barriers obtained from periodic density functional calculations. We considered three possible mechanisms encompassing four different intermediates, ethyl, vinyl, ethylidene, and vinylidene. Our simulations predict that the most plausible pathway on both surfaces is ethylene --> vinyl --> vinylidene --> ethylidyne. In contrast to earlier suggestions that the dehydrogenation to vinyl is rate-limiting on Pt(1 1 1), we found the hydrogenation of vinylidene to ethylidyne to be crucial on this surface. On Pd(1 1 1), the initial dehydrogenation of ethylene is rate-limiting. Hence, vinylidene species accumulate on Pt(1 1 1), while all intermediates on Pd(1 1 1) convert rapidly to ethylidyne without accumulation. The simulated apparent activation energies for the formation of ethylidyne on Pd(1 1 1), 94 kJ mol(-1), and on Pt(1 1 1), 65 kJ mol(-1), agree well with experimental results. (C) 2011 Elsevier Inc. All rights reserved.