Angewandte Chemie
Eine Zeitschrift der Gesellschaft Deutscher Chemiker

Supporting Information

69451 Weinheim, Germany

Hydrocarbon Chain Growth on V(100) Single-Crystal Surfaces Via Vinyl Intermediates

Min Shen and Francisco Zaera*

Department of Chemistry, University of California, Riverside, California, CA, 92521, USA

Supporting Information

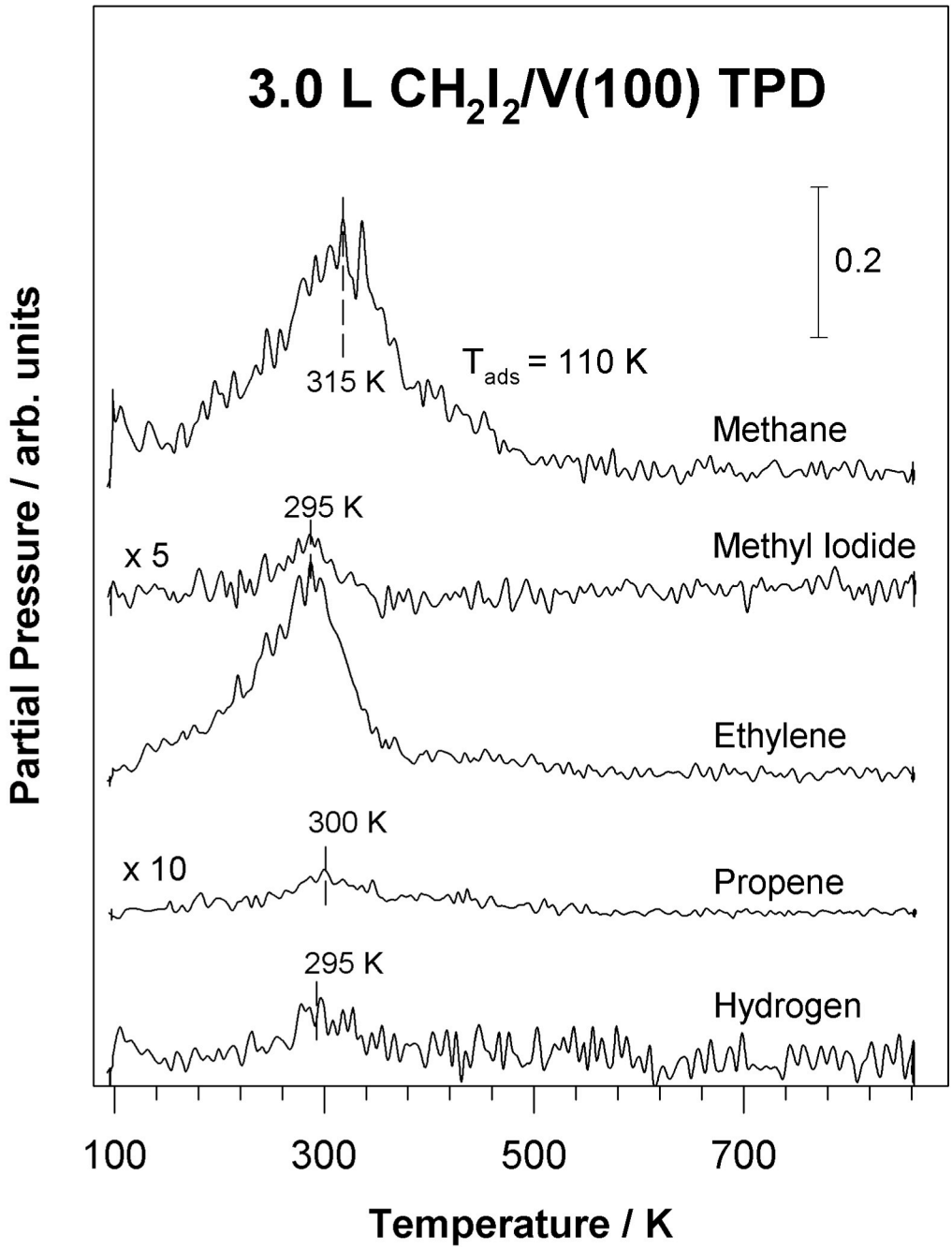

Figure S1. TPD spectra from 3.0 L of diiodomethane adsorbed on a clean V(100) surface. Heating rates of 10 K/s were used in all TPD experiments in this paper. The main products detected in this system are hydrogen, methyl iodide, methane, ethene, and propene. No ethane, propane, or 1,3-butadiene are observed.

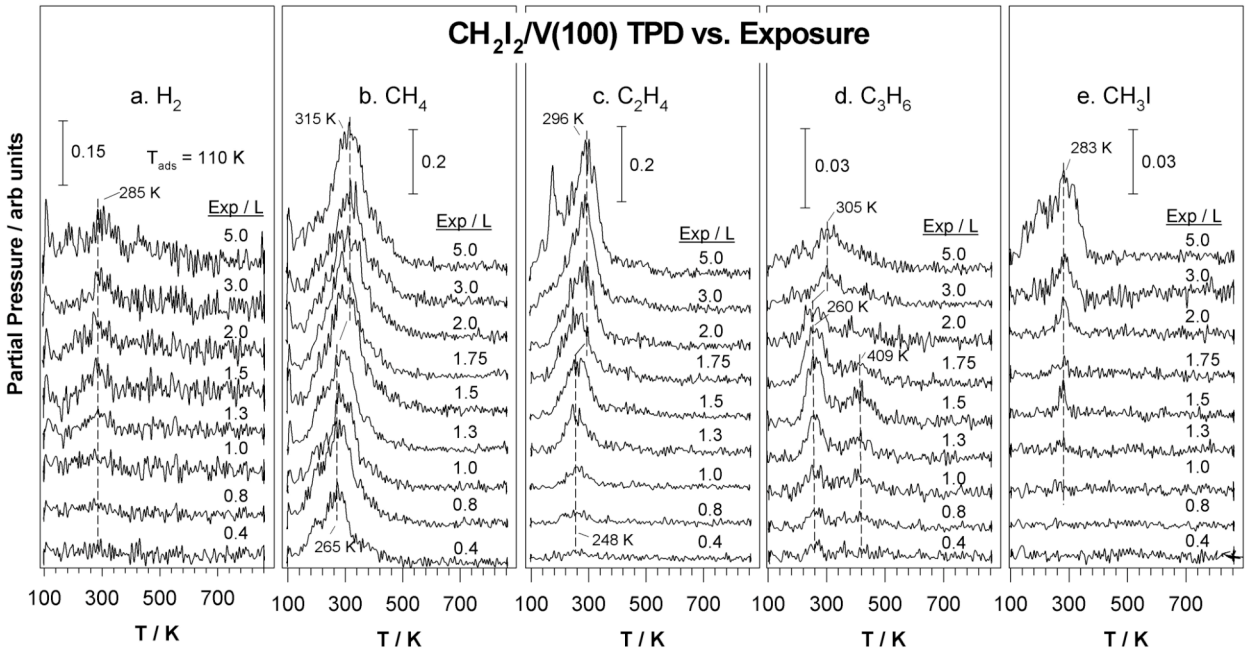

Figure S2. H_2 (a), CH_4 (b), C_2H_4 (c), C_3H_6 (d), and CH_3I (e) TPD spectra from diiodomethane adsorbed on clean V(100) as a function of initial dose. Methane production is dominant at low CH_2I_2 coverages, but ethene production becomes competitive at high CH_2I_2 coverages. Propene desorption shows up in two peaks, and its yield is optimized at intermediate CH_2I_2 coverages. Molecular desorption, together with some CH_3I, is seen only after CH_2I_2 exposures above 3.0 L.

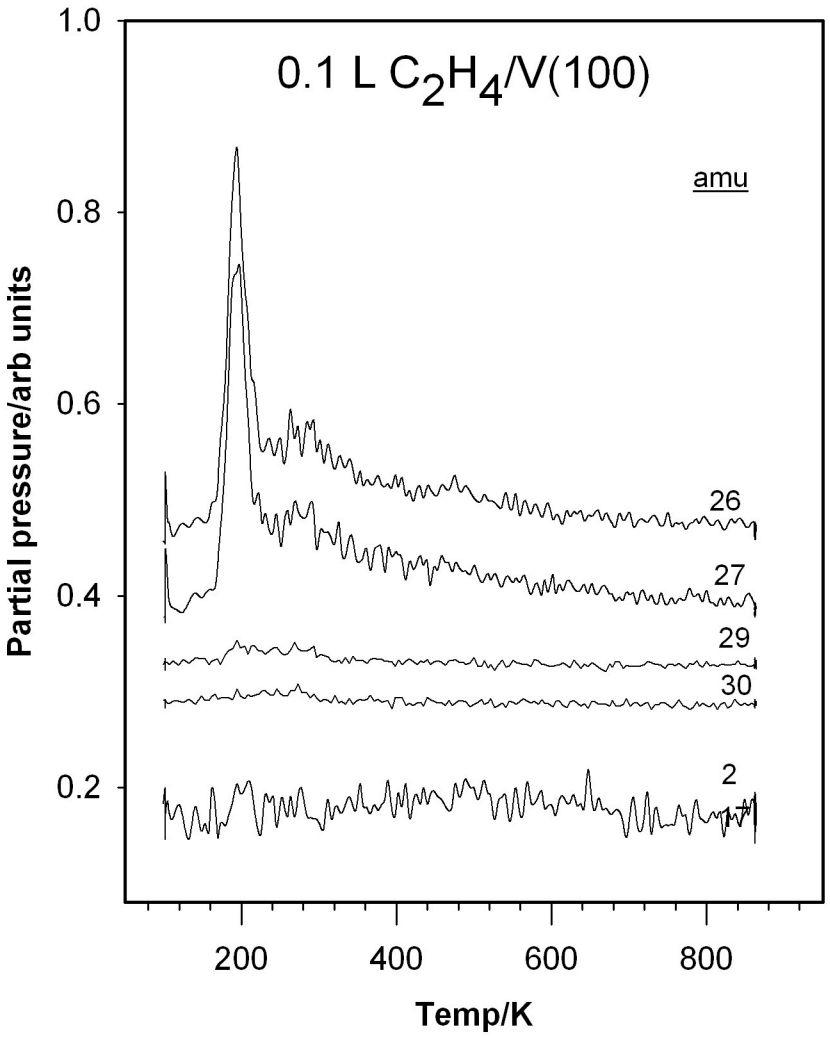

Figure S3. TPD spectra from 0.1 L of ethene adsorbed on a clean V(100) surface. The traces for 26 and 27 amu reflect molecular desorption from the monolayer around 200 K, indicating weak adsorption. The absence of signals for 29 and 30 amu rule out any hydrogenation to ethane. Virtually no hydrogen (2 amu) desorption is seen either, so no significant dehydrogenation occurs with this adsorbate.

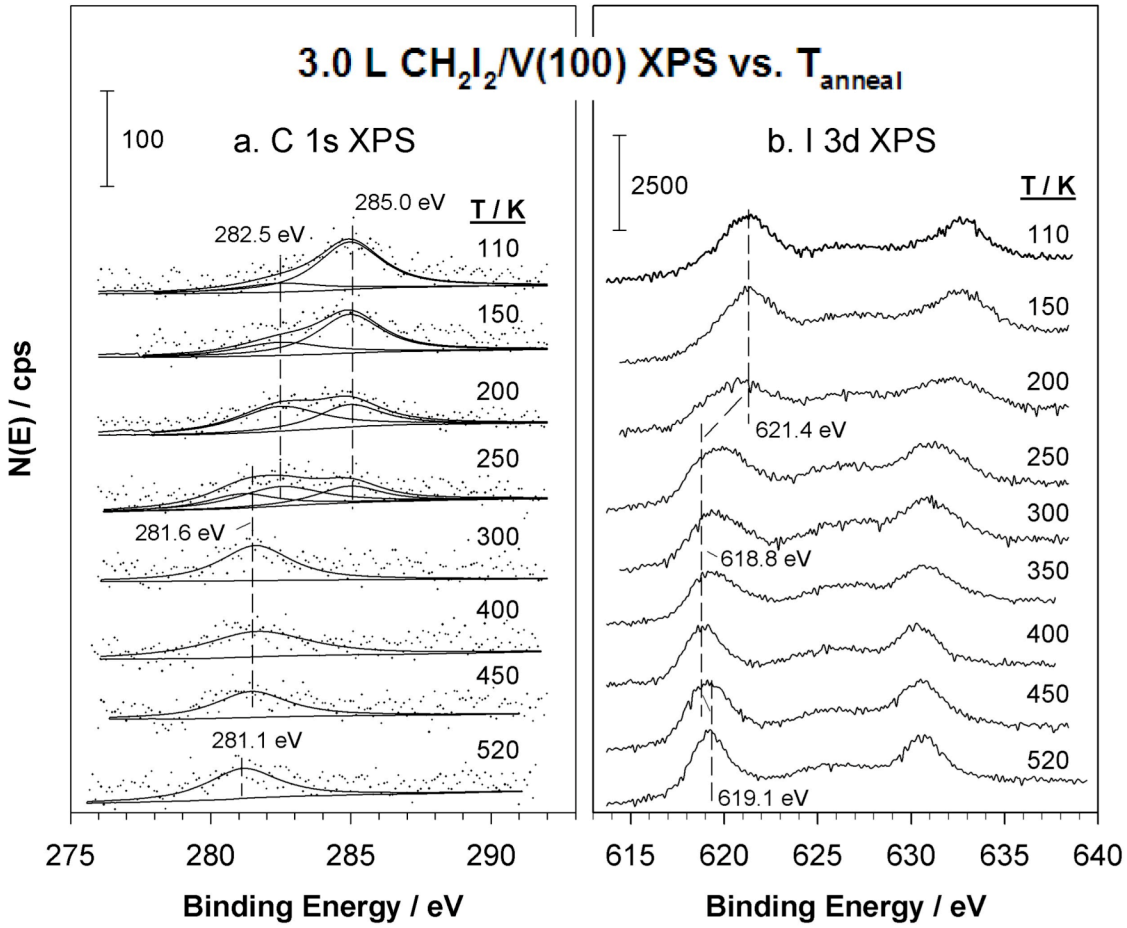

Figure S4. C 1s (left panel) and I 3d (right panel) XPS spectra for 3.0 L of adsorbed CH_2I_2 on clean V(100) surfaces as a function of annealing temperature. The peaks for C 1s and I $3d_{5/2}$ seen below 250 K at 285.0 and 621.4 eV, respectively, correspond to molecular CH_2I_2. Heating to temperatures above 200 K leads to the thermal dissociation of the C–I bonds as shown by the initial shifts in both I 3d and C 1s XPS peaks at 250 K. Dehydrogenation of the resulting surface hydrocarbon species is inferred by the further peak shift seen in the C 1s XPS spectra around 300 K.

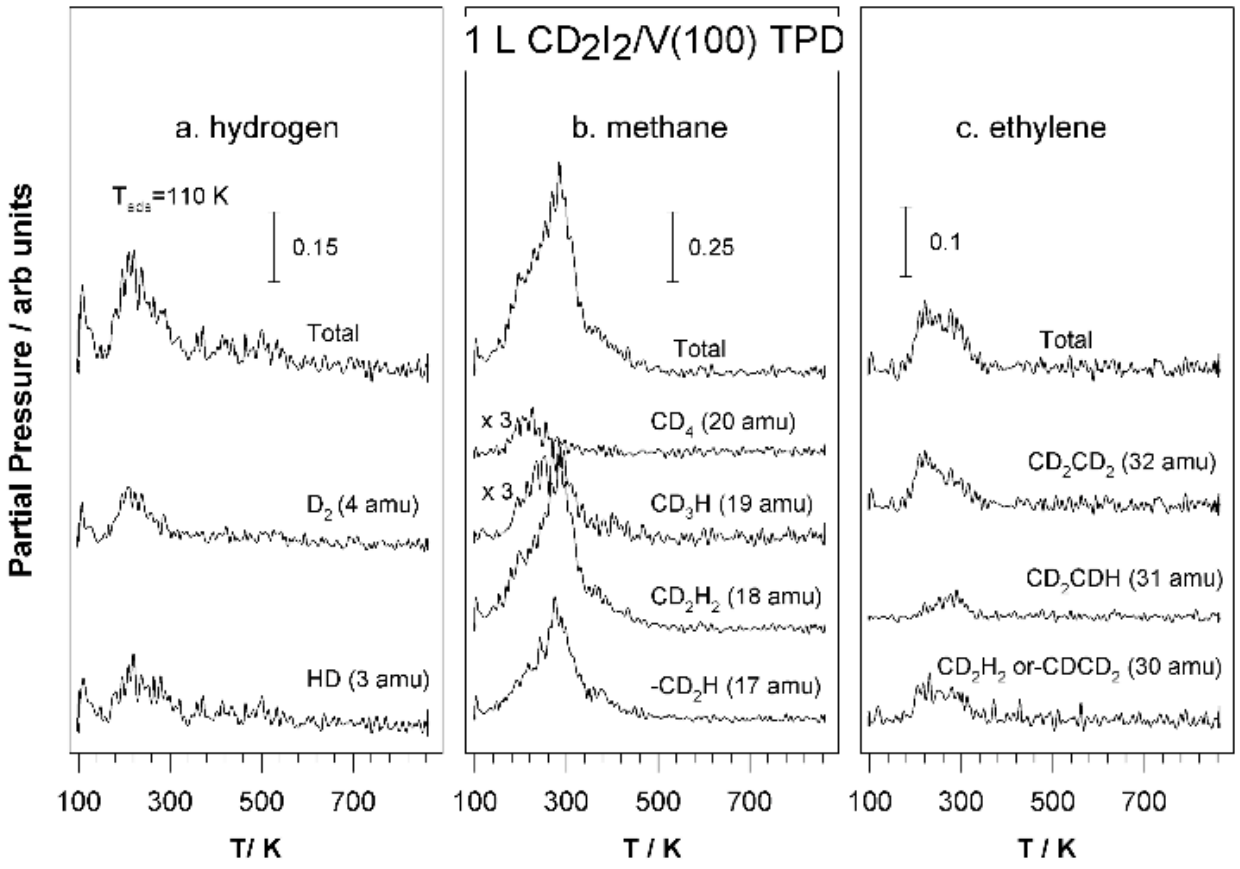

Figure S5. TPD spectra from 1.0 L of perdeuterodiiodomethane adsorbed on a clean V(100) surface. Left panel: hydrogen (HD and D_2) desorption traces indicating dehydrogenation (dedeuteration) of the surface methylene moieties above 200 K. Middle panel: Methane formation, mainly in the form of CD_2H_2. The small amounts of CD_4 and CD_3H detected are indicative of the limited extent to which the original perdeuteromethylene surface moieties undergo dehydrogenation (dedeuteration). Right panel: ethene formation. The majority of this product evolves in the form of CD_2CD_2, but the detection of significant amounts of CD_2CDH do point to previous dehydrogenation (of methylene to methylidyne).