Supplementary Information

Structure of chemisorbed 1,3-butadiene on the Cu(111) surface

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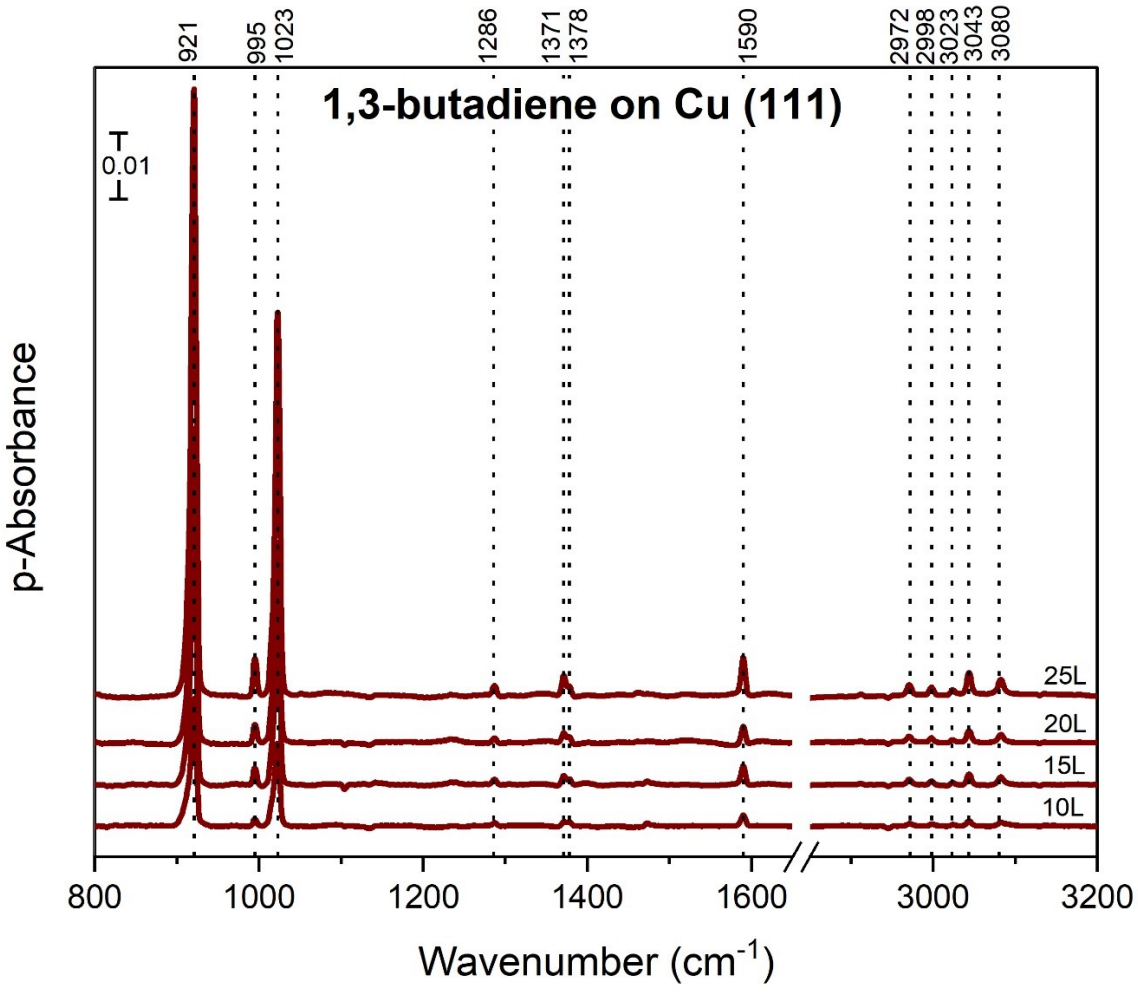

Figure S1. RAIR spectra for multilayer 1,3-butadiene obtained after 10, 15, 20, and 25 L exposures.

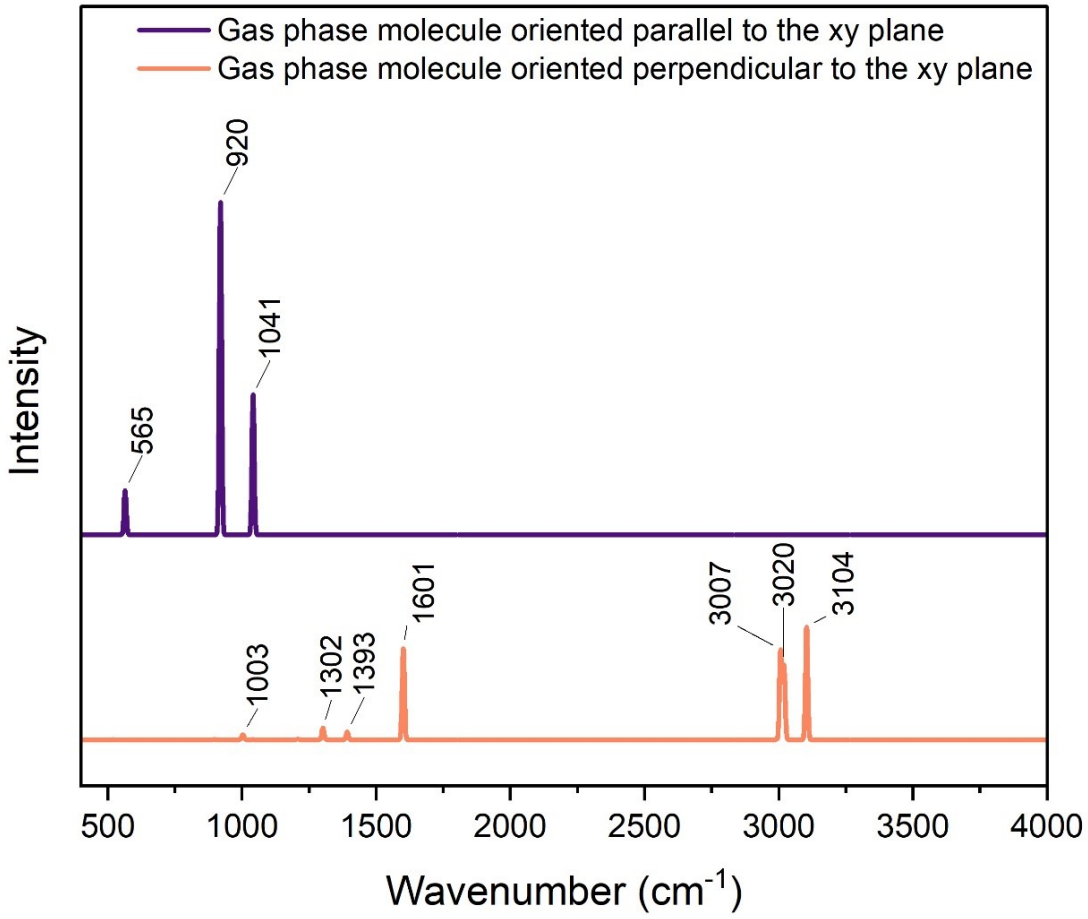

Figure S2. Calculated RAIR spectra for 1,3-butadiene oriented with the molecular plane parallel to the Cu(111) surface but not interacting with it. The out-of-plane modes (purple) are surface IR allowed, whereas the in-plane modes (orange) are forbidden.

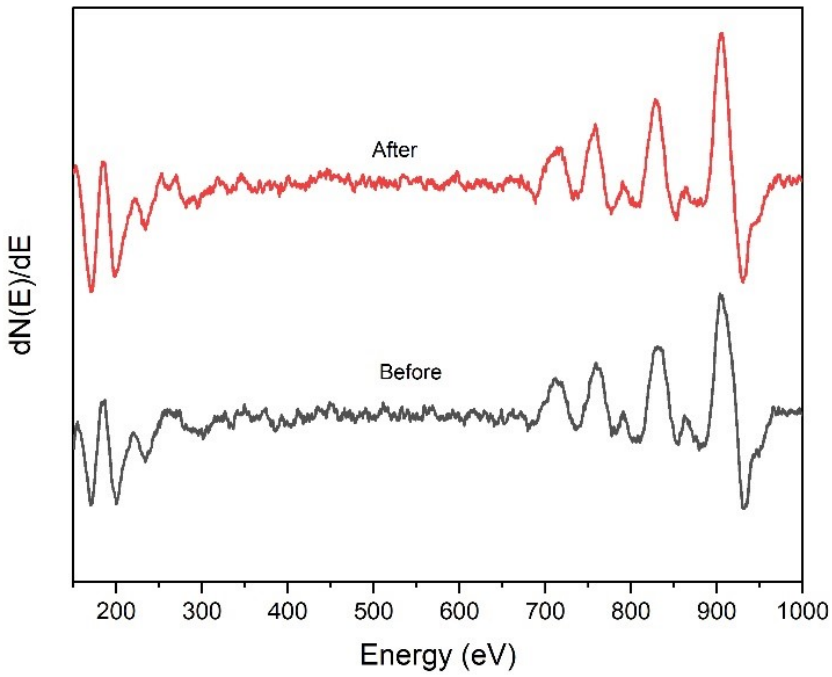

Figure S3. Auger electron spectra obtained with an electron beam energy of 2.5 keV for the clean Cu(111) surface (black) and after desorption of 1,3-butadiene following an exposure of 5.0 L with the crystal at 85 K.

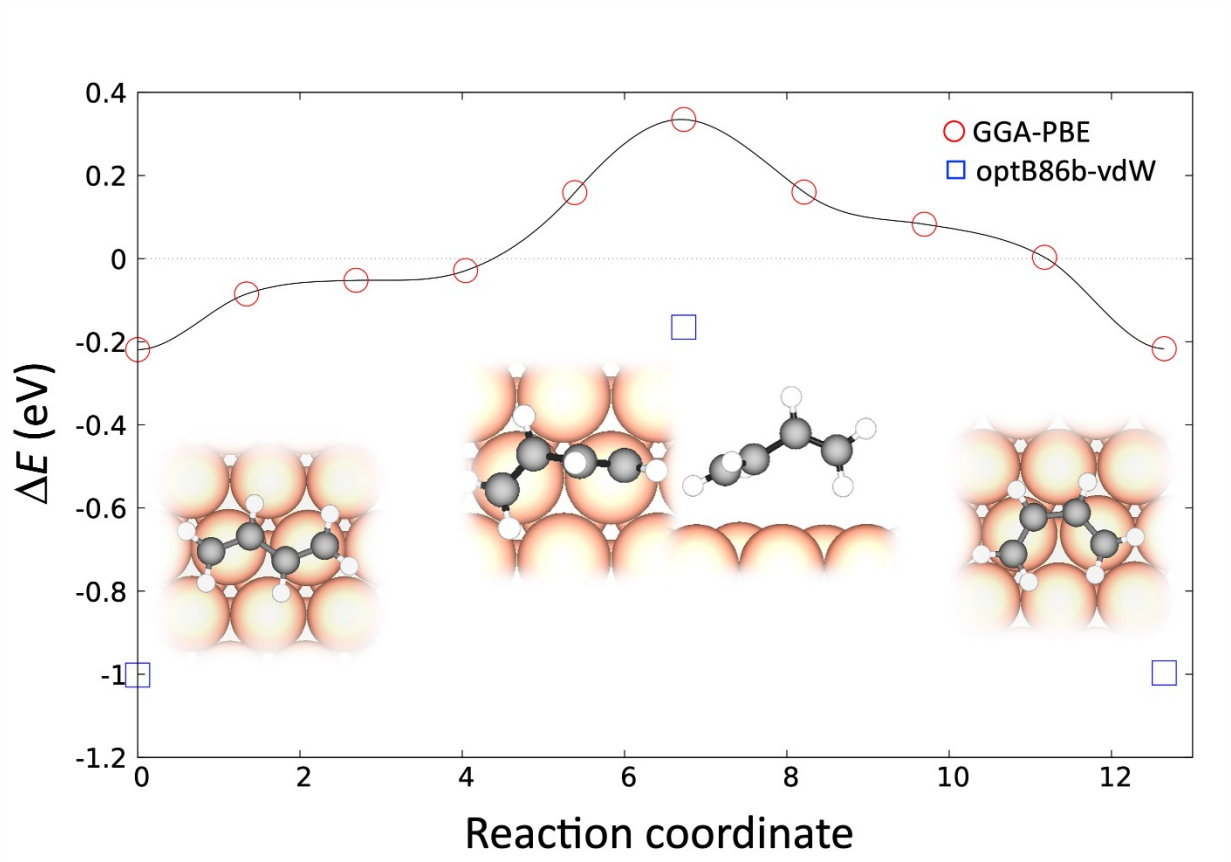

Figure S4. GGA-PBE minimum-energy reaction pathway for isomerization between the *s-trans* and *s-cis* di-π isomers of 1,3-butadiene. The images used in the CI-NEB calculation are indicated by circles. The corresponding IS, TS, and FS of the same reaction calculated using optB86b-vdW are indicated by squares below the corresponding GGA-PBE states and their configurations are shown in the insets. Zero on the energy axis corresponds to 1,3-butadiene in the gas phase.