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Furan Decomposition Mechanism on Vicinal Pd(111) Studied by STM and DFT[1] A. LOUI, University of California Davis, C. Y. FONG, University of California Davis, S. CHIANG, University of California Davis — We have used scanning tunneling microscopy to investigate the behavior of furan (C_4H_4O) adsorbed on stepped Pd(111) at 199 and 225 K, as well as aspects of its decomposition after heating to a maximum temperature of 415 K. Studies conducted on two substrates with relatively narrow and wide terraces show that furan preferentially adsorbs at step edge sites on both surfaces, while evidence of molecular diffusion is seen only on the narrower vicinal planes. After heating to 288 K, 300 K, and 415 K, evidence of reaction can be observed in occupied-states STM images. Our observations support a furan decomposition mechanism wherein the heterocycle preferentially adsorbs and reacts at upper step edge sites. Ab initio calculations based on Hohenberg-Kohn density functional theory (DFT) have been performed for several high-symmetry adsorption sites of furan on flat Pd(111) and show distortions of both the furan and the top layer of Pd upon adsorption.

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