

Abstract Submitted
for the CAL11 Meeting of
The American Physical Society

Adsorption and desorption mechanisms for allylamine, propylamine, propylchloride, and propylene on the Si(100)-2x1 surface LEKH ADHIKARI, SEAN CASEY, University of Nevada, Reno — The mechanisms for adsorption and desorption of allylamine, propylamine, propylchloride, and propylene on the Si(100)-2x1 surface has been investigated experimentally using thermal desorption spectroscopy (TDS) and computationally using density functional theory (DFT) calculations. TDS was carried out to track down possible desorption products and their desorption temperatures and DFT calculations were done to help elucidate the experimental results, and to more fully probe mechanistic pathways consistent with the TDS results. All of these molecules are three carbon chain moieties with differing terminal functional groups and were chosen to self-consistently probe amine and alkene functional group chemistry on this surface. Results from the adsorption of propylene and allylamine were mostly consistent with previous studies on adsorption of these molecules, with the main difference being the observation of a prominent $m/z = 17$ desorption product in the case of TDS after allylamine adsorption. TDS after propylamine and allylamine adsorption gave rise to a prominent propylene ($m/z = 42$) desorption channel. The TDS results showed that propylene and halo-alkanes such as chloro-propane also display a propylene desorption channel, but it appears at a lower surface temperature than for the amines. This is an indication that the amine adsorption and decomposition mechanisms is different than halo-alkane or alkene reaction on the Si(100)-2x1 surface, in that it does not involve any silicon-carbon bond forming reactions initially. This is consistent with the computational results as well.

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Date submitted: 10 Oct 2011

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