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Alanes formation on the Al(111) surface SYLVIE RANGAN, JEAN-FRANCOIS VEYAN, YVES J. CHABAL, University of Texas at Dallas, SANTANU CHAUDHURI, Washington State University, JAMES T. MUCKERMAN, Brookhaven National Laboratory — Alane clusters (Al_xH_y) are believed to be the ubiquitous intermediates in hydrogen storage reactions for a wide variety of alanates (LiAlH_4 , NaAlH_4) currently considered for hydrogen storage. The formation and behavior of alanes at surfaces appear to control and limit the efficiency of hydrogen storage. In particular, hydrogen adsorption on the Al(111) surface leads to the coexistence of several adsorbed species, the concentration of which is affected by the step density, the surface coverage and the temperature. We combine density functional theory (DFT) and surface infra-red (IR) absorption spectroscopy to uncover the mechanisms for alane formation on Al(111) surfaces. At low coverage, DFT predicts a two-fold bridge site adsorption for atomic hydrogen, consistent with previous Electron Energy Loss Spectroscopy measurements. At higher coverage, the formation of small chemisorbed AlH_3 occurs at the step edges. With increasing coverage AlH_3 is extracted from the step edge and becomes highly mobile on the terraces in a weakly bound state. This mobility is the key factor leading to the growth of larger alanes through AlH_3 oligomerization. For these large alanes, previous Thermal Programmed Desorption studies are discussed and compared to the thermal stability observed in IR.

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