Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Defect-mediated Alane formation on Ti-doped Al(111) surfaces: a DFT study ADITI HERWADKAR, LIN-LIN WANG, DUANE D. JOHNSON, Ames Laboratory/US Department of Energy, Iowa State University — Understanding of Alane (AlH_3) formation on Al surface remains elusive, including interpreting STM results under various conditions. Using density functional theory calculations, we study Alane formation on close-packed (111) and stepped surfaces with {111} and {100} microfacets of Al, with and without Ti as a catalyst. We find that Ti dopants act as catalyst in the formation of Alane on Al(111) via a vacancy-mediated mechanism. Additionally, we find the Alane formation energy at steps is 40% less than that from the flat surface. We assess the energetics of various surface-defect configurations to understand the concerted roles that Ti dopants, surface vacancies, and step defects play in Alane formation. Work was supported in part by Department of Energy, Office of Basic Energy Science under contract DEFC36-05GO15064 (Sandia Metal-Hydride Center of Excellence), DE-FG02-03ER15476, DE-FG02-03ER46026, and DE-AC02-07CH11358 at the Ames Laboratory operated by Iowa State University.

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Date submitted: 14 Dec 2010 Electronic form version 1.4