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Molecular hydrogen interaction with Ti doped Al(111) surfaces
IRINDER CHOPRA, University of Texas at Dallas, SANTANU CHAUDHURI, Washington state University, JEAN-FRANCOIS VEYAN, YVES CHABAL, University of Texas at Dallas — Alanates are promising hydrogen storage materials, but have poor re-hydrogenation kinetics. Decomposition[1] of $NaAlH_4$ can be made reversible at reasonable temperatures and pressures by adding titanium. There is however little understanding of the role of Ti as a catalyst,[2] and no experimental evidence for H_2 dissociation on Ti-doped Al surfaces. Using CO as a probe molecule in conjunction with in-situ infrared absorption spectroscopy, we present unambiguous evidence for molecular hydrogen dissociation, chemisorptions and spill over on with Ti doped Al(111) surfaces. The optimum catalytic activity of the Ti-doped Al surface occurs for a Ti coverage of 0.1 monolayer. At high hydrogen coverage, no CO physisorption is observed, indicating that the dissociated hydrogen spill over from the catalytic active Ti site. CO molecules can be chemisorbed at the catalytic sites but do not spill over. These findings provide important information on the nature of the catalyst during the hydrogenation reactions.

[1] *J. Alloys Compd.* 1997, 253, 1.
[2] *J Am Chem Soc* 2006, 128, (35), 11404-11415.

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