Atomic and Molecular Hydrogen Interaction with Ti-Doped Al (100): Hydrogen Dissociation and Surface Alane Formation

ERIK MULLER, PETER SUTTER, PERCY ZAHL, Center for Functional Nanomaterials, Brookhaven National Laboratory, SANTANU CHAUDHURI, JAMES MUCKERMAN, Department of Chemistry, Brookhaven National Laboratory — A comprehensive research effort on the atomistic mechanisms underlying hydrogen storage in Ti-doped NaAlH$_4$ is aimed at deriving a knowledge base for the rational optimization of this and other related complex hydride materials. Our investigation focuses on the role of the Ti dopants in promoting reversible hydrogenation, a key requirement for any practical hydrogen storage material. The re-hydrogenation reaction proceeds from the crucial initial step of dissociative adsorption of molecular hydrogen on Al or NaH. A specific Al:Ti complex was recently predicted as an active site for H$_2$ dissociation on extended Al(100) surfaces [1]. Combining high-resolution surface imaging experiments (scanning tunneling microscopy, low-energy electron microscopy) with density functional theory, we are investigating the dissociative adsorption of H$_2$ on Ti-doped Al(100) prepared in ultrahigh vacuum. We will discuss our progress toward identifying catalytically active sites for H$_2$ dissociation on this surface, as well as pathways toward the formation of mobile Al-species. [1] S. Chaudhuri and J.T. Muckerman, J. Phys. Chem. B 109, 6952 (2005).