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Effect of Ti Dopant on Surface Diffusion of Isolated Alane Species: A Comparison between Al (111) and Al (100) surfaces[1] ALTAF KARIM, JAMES MUCKERMAN, Brookhaven National Lab — Our density functional theory-based kinetic Monte Carlo simulations show that an embedded Ti atom creates a well in the potential energy surfaces of Al(111) and Al(100) as probed by hydrogen and other isolated alane species. Hydrogen adatoms become trapped around Ti atoms on an Al(111) surface, whereas Al adatoms do not exhibit any significant effect of the potential energy well created by the Ti atoms. In contrast to the case of Al(111), Al adatoms on an Al(100) surface also become trapped around the Ti atoms for a longer period of time compared to the hydrogen adatoms on this surface. Therefore, Ti sites on Al(100) become poisoned by the presence of Al adatoms around them for long periods of time, thereby blocking further dissociative adsorption of hydrogen. The overall diffusion of Al adatoms on an Al(100) surface is significantly lower compared to the Al(111) surface. This fact suggests that the Ti-doped Al(111) surface is perhaps more conducive to the production of alane species than the Ti-doped Al(100) surface despite its higher activation barrier for the dissociation of molecular hydrogen.

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