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Multiscale modelling of Interaction of Alane Clusters on Al(111) surface: A Reactive Force Field and Infrared Absorption Spectroscopy Approach JULIUS OJWANG, Carnegie Geophysical Laboratory, ADRI VAN DUIN, Penn State, WILLIAM GODDARD III, Caltech, RUTGER VAN SANTEN, Eindhoven University of Technology — Alanes are believed to be the ubiquitous facilitators of mass transport of aluminum atoms during the thermal decomposition of $NaAlH_4$. Alanes also take part on decomposition of AlH_3, another important material for hydrogen storage. We have used interplay of theoretical simulations (reactive force field and density functional theory) and experiments (IR reflection absorption spectroscopy) to address the issue of the role of alanes as facilitators of mass transport of aluminum atoms. We have obtained valuable details on the mechanism of formation and agglomeration of alanes on Al(111) surface. Our simulations show that, on the Al(111) surface, alanes oligomerize into larger alanes. The identification of these string like intermediates as a precursor to the bulk hydride phase allows us to explain the loss of resolution in surface IR experiments with increasing hydrogen coverage on single crystal Al(111) surface. This is in excellent agreement with the experimental works of Go et al. (E. Go, K. Thuermer, J.E. Reutt-Robey, Surf. Sci.,437:377(1999)).

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