ニューラルネットワークポテンシャルを用いたトリメチルアルミニウム吸着状況の解析

Adsorption state study of Trimethylaluminum using neural network potential

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Atomic Layer Deposition (ALD) is primarily applied in semiconductor fabrication due to its characteristics of alternately supplying the precursor gas and reaction gas, relying on surface saturation adsorption of the precursor gas. This results in excellent uniformity in both macro and microfilm thickness and stability against fluctuation of fabrication conditions. To achieve an ideal ALD process with these properties, it is crucial to carefully select the precursor and reaction gases, along with the optimal reaction conditions. Efficient process development can be achieved by determining the best process parameters by analyzing adsorption equilibrium states derived from adsorption, desorption, and surface reaction studies. Conventional computation methods like Density Functional Theory (DFT) provide opportunities to examine surface adsorption and reaction of precursors. However, analyzing such mechanisms is costly in time by DFT and is extremely time-consuming to predict the effect of steric hindrance effect on the adsorption of multiple precursors (especially for large metalorganics) because of the inevitable large dimensions of the simulation system (slab size). However, we are using a state-of-the-art atomic-level simulator (Matlantis^{TM}) to explore the adsorption and reaction of Trimethylaluminum (TMA) for Al_2O_3 ALD with H_2O as the reactant. It could easily predict the adsorption behavior of precursors on large adsorption surfaces with an extremely short time in scales of minutes, due to the precise neural network potential developed by advanced machine-learning-based technique. We calculate the adsorption mechanism and growth for TMA by Matlantis^{TM} and figure out it has good agreement with previous DFT calculations and QCM experiments results.

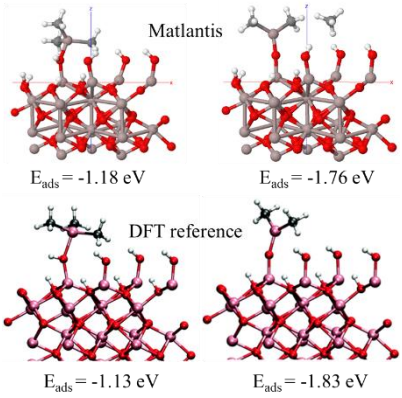

Fig.1 TMA adsorption comparison by Matlantis^{TM} and DFT

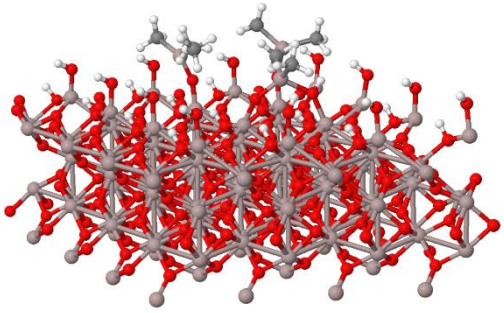

Fig.2 Three TMA molecules adsorption structure with steric hindrance effect by Matlantis^{TM}