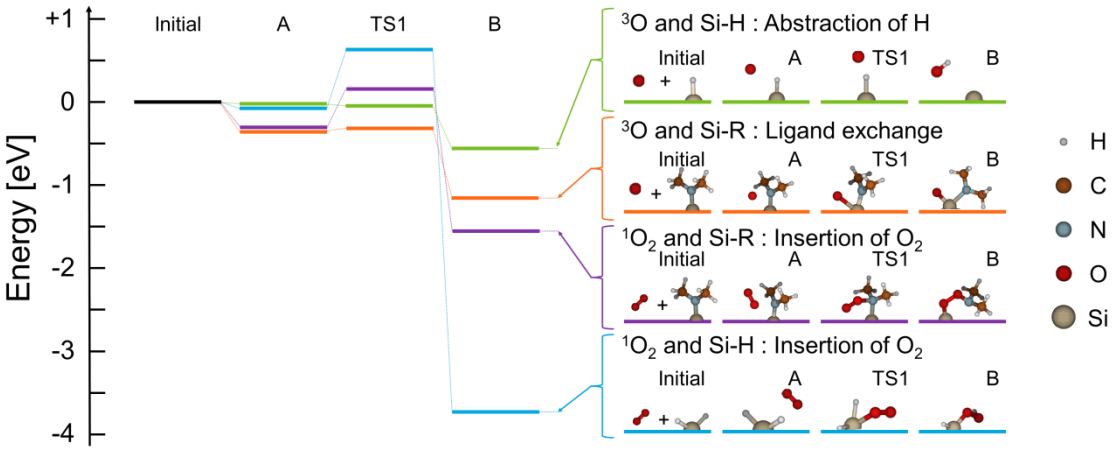


Figure 1. Comparison of energy barriers according to oxidation pathways by DFT study with CAM-B3LYP/6-311++g(d,p) basis sets. State A and B represent intermediate state of each reaction. Transition state between A and B is shown in TS1. No barriers were observed only in $^3$O oxidation paths as shown in green and orange lines, which are expected to dominate as the surface reactant at very low process temperature.

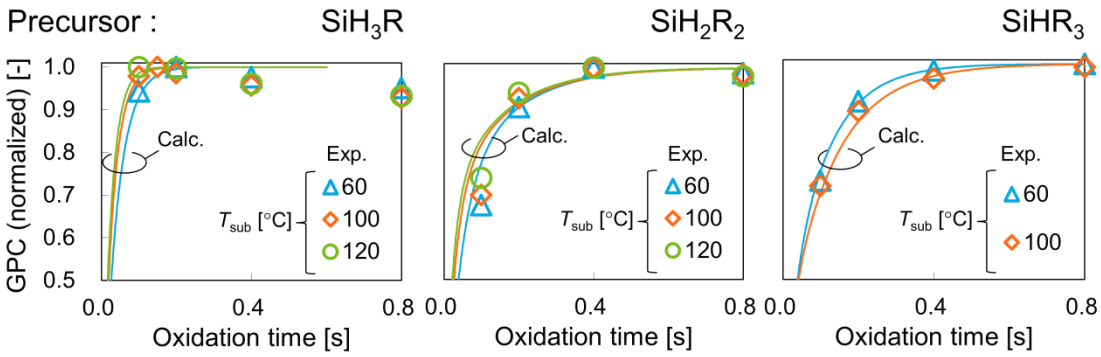


Figure 2. Comparison between experimental results for normalized growth per cycle (GPC) with calculation results from our surface oxidation model. Saturation trends for these various cases can be explained well by a two oxidation rate model; oxidation of Si-H bonds and Si-R bonds.