Supporting Information:

Accelerated Deep Learning Dynamics for Atomic Layer Deposition of Al(Me)$_3$ and Water on OH/Si(111)

Hiroya Nakata,[*] Michael Filatov(Gulak),[*] and Cheol Ho Choi[*]

Department of Chemistry, Kyungpook National University, Daegu 41566, South Korea

E-mail: nakata.hiro07@gmail.com; mike.filatov@gmail.com; cchoi@knu.ac.kr

List of Figures

List of Tables

Reaction Coordinate for TDUS

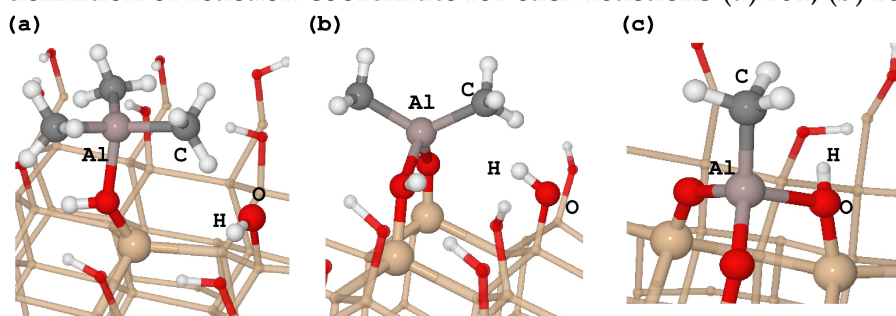Label for definition of reaction coordinate for each reactions (a) r01, (b) r02, (c) r03,

Table S1: Definition of reaction coordinate

	R (r01)	P (r01)	R (r02)	P (r02)	R (r03)	P (r03)
Al-O	4.127	1.813	3.785	1.805	1.950	4.250
O-H	1.000	2.428	0.980	2.389	3.324	1.108
H-C	3.681	1.112	2.111	1.105	1.015	2.985
C-Al	1.991	4.003	1.985	4.253	2.006	1.753

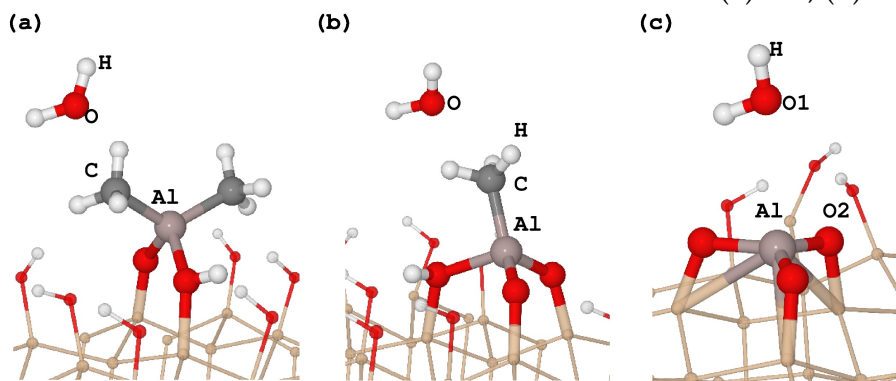Label for definition of reaction coordinate for each reaction (a) r04, (b) r05, (c) r06

Table S2: Definition of reaction coordinate for r04 and r05

	R (r04)	P (r04)	R (r05)	P (r05)
Al-C	1.969	5.028	1.949	5.817
C-H	4.385	1.104	6.895	1.105
H-O	0.967	2.544	0.966	3.062
O-Al	4.816	1.779	7.700	1.714

Table S3: Definition of reaction coordinate for r06

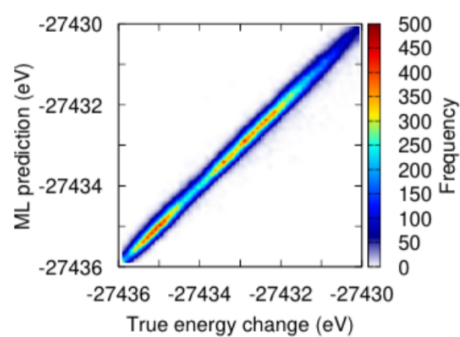|	R (r06)	P (r06)
Al-O1	3.746	1.711
O1-H	0.972	2.869
H-O2	4.048	0.977
O2-Al	1.744	1.958
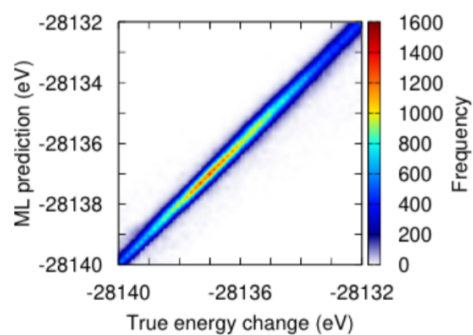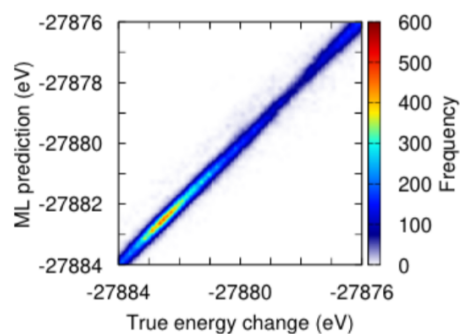
Figure S1: Comparison between DFT energy and energy estimated by ML force field for (a) Reaction from Figure **??**-(a) of the main text. (b) Reaction from Figure **??**-(b) of the main text. (c) Reaction from Figure **??**-(c) of the main text.
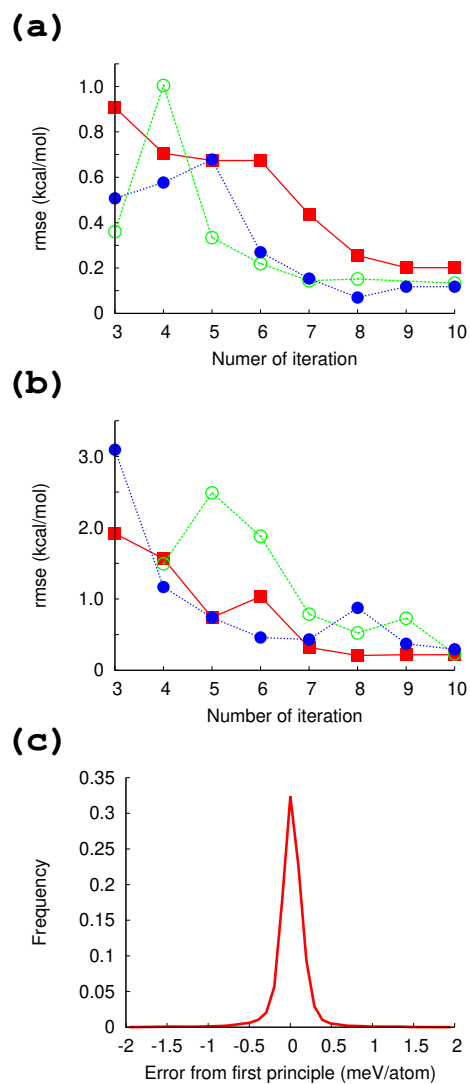
(a)

(b)

(c)

Figure S2: (a) CH$_4$ evolution reaction, red, Green, and blue denote reaction r01, r02, and r03, respectively. (b) water splitting reaction, red, green, and blue denote reaction r04, r05, and r06, respectively. (c) Evaluation of energy difference between ML force field and first principle simulation.