Supplemental Information

As shown in Fig. 1(a), $Pd(hfac)_2$ does not chemisorb on the OH-terminated SiO_2 surface even after 1000 ps of MD. In contrast, rapid chemisorption is observed on the OH-terminated Al_2O_3 surface within 25 ps, as shown in Fig. 1(b-1). However, no chemisorption occurs on the gibbsite-like OH-terminated Al_2O_3 surface shown in Fig. 1(b-2), even after 1000 ps, similar to the behavior on SiO_2.

Figure 2 shows the Pd amount after Pd-ALD using $Pd(hfac)_2$ on substrates subjected to different surface treatments. Pd loading increases on SiO_2 after treatment, whereas on Cu a significant increase is observed only when the additional H_2O treatment in condition (c) is applied. The lower effectiveness of condition (b) compared with (c) is attributed to the formation of a gibbsite-like Al_2O_3 surface.

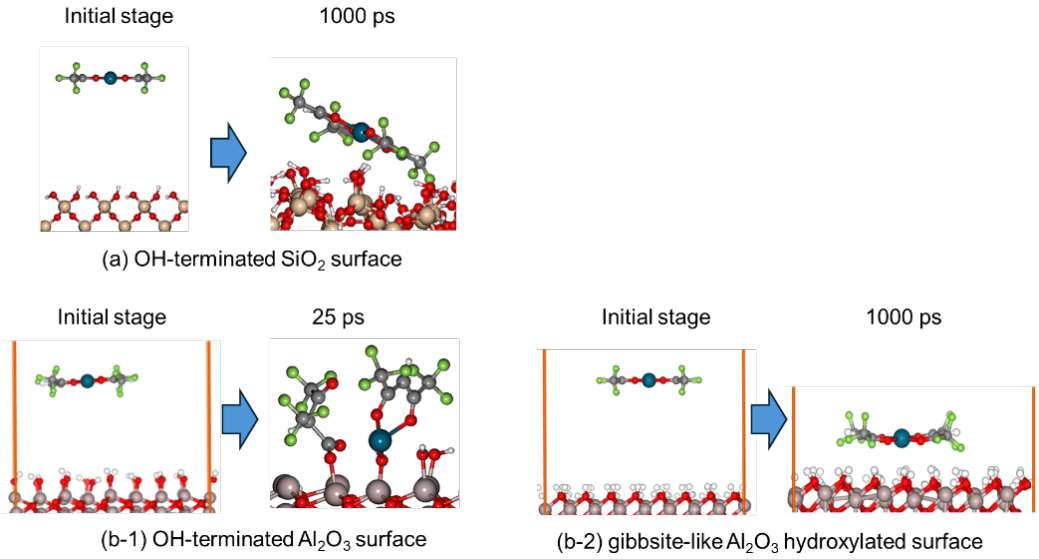

Fig. 1. Adsorption of $Pd(hfac)_2$ on OH-Terminated Surfaces. (a) SiO_2, (b-1) Al_2O_3, (B-2) gibbsite-like Al_2O_3.
Chemisorption of $Pd(hfac)_2$ is observed on the OH-terminated Al_2O_3 surface (b-1), whereas no adsorption is observed on the SiO_2 surface (a) or on the gibbsite-like Al_2O_3 surface (c).

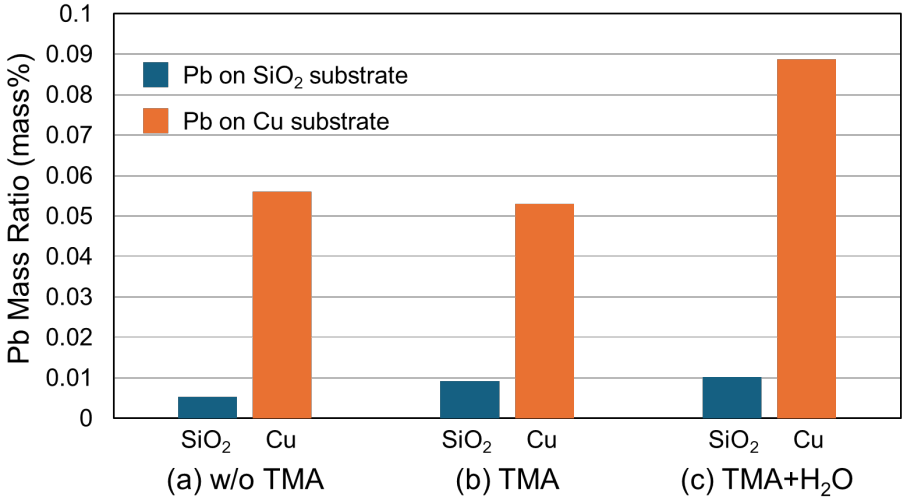

Fig. 2. Pd Mass Fraction after Pd-ALD with Different TMA Treatments (WD-XRF).
The chemisorption of $Pd(hfac)_2$ was enhanced by TMA treatment.