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Supplementary Information

High-temperature atomic layer deposition of HfO_2 film with low impurity using a novel Hf precursor

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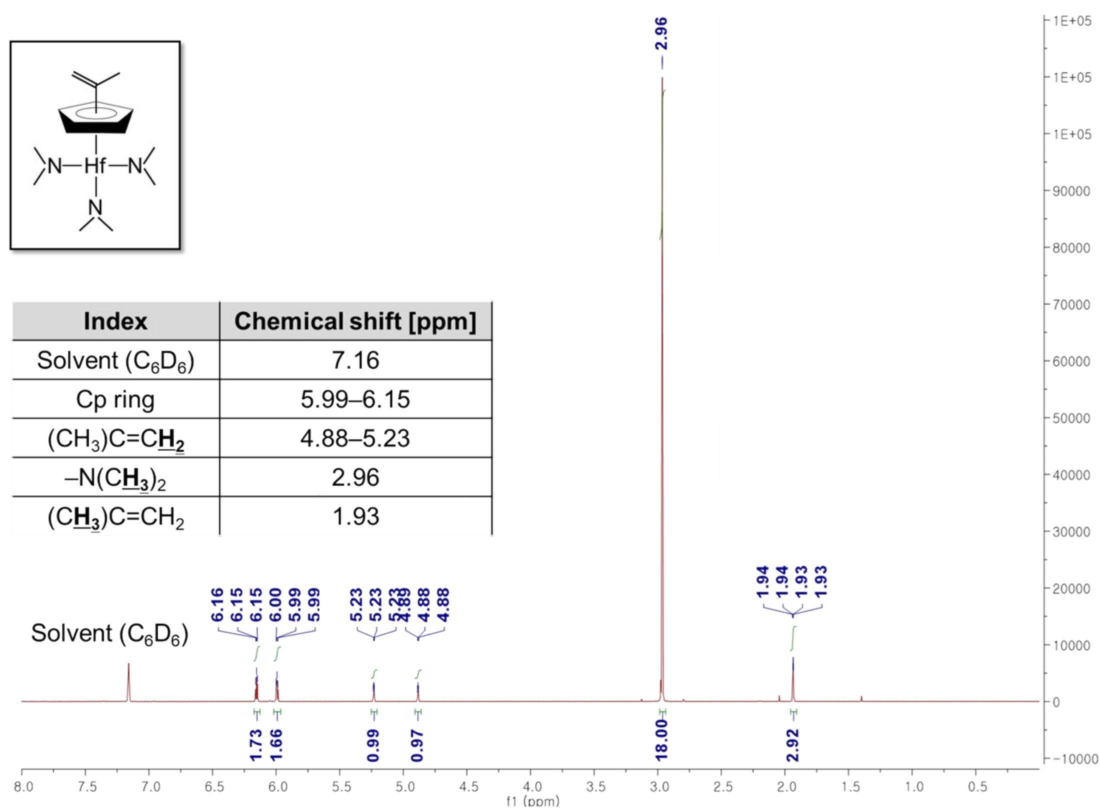

Index	Chemical shift [ppm]
Solvent (C_6D_6)	7.16
Cp ring	5.99–6.15
$(CH_3)C=C\underline{\mathbf{H_2}}$	4.88–5.23
$–N(C\underline{\mathbf{H_3}})_2$	2.96
$(C\underline{\mathbf{H_3}})C=CH_2$	1.93

Fig. S1 ^1H NMR spectrum of $FuHf(NMe_2)_3$ precursor

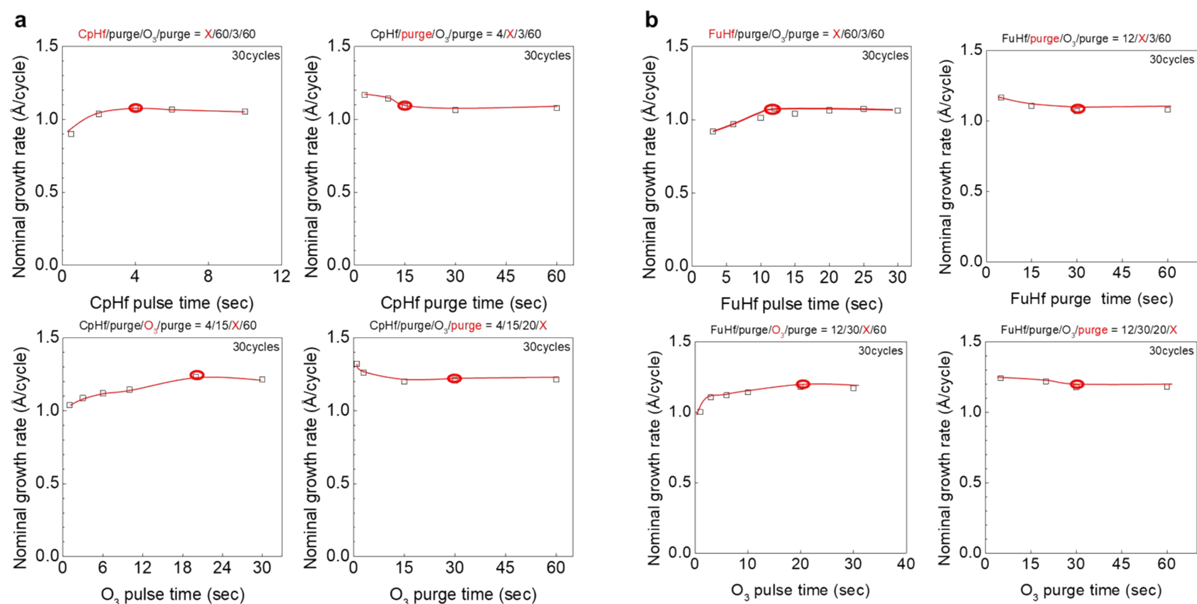

Fig. S2 Nominal growth rates of the HfO_2 films grown using (a) CpHf and (b) FuHf precursors as a function of the precursor pulse/purge time and reactant pulse/purge time.

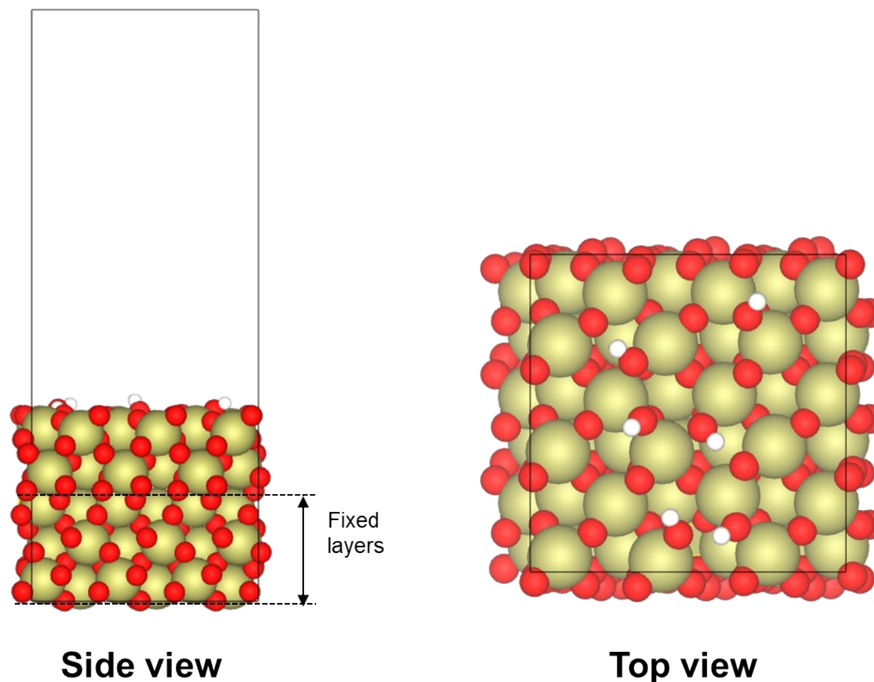

Fig. S3 The monoclinic HfO_2 (001) surface model used in this work. (green = Hf, red = O, white

= H)

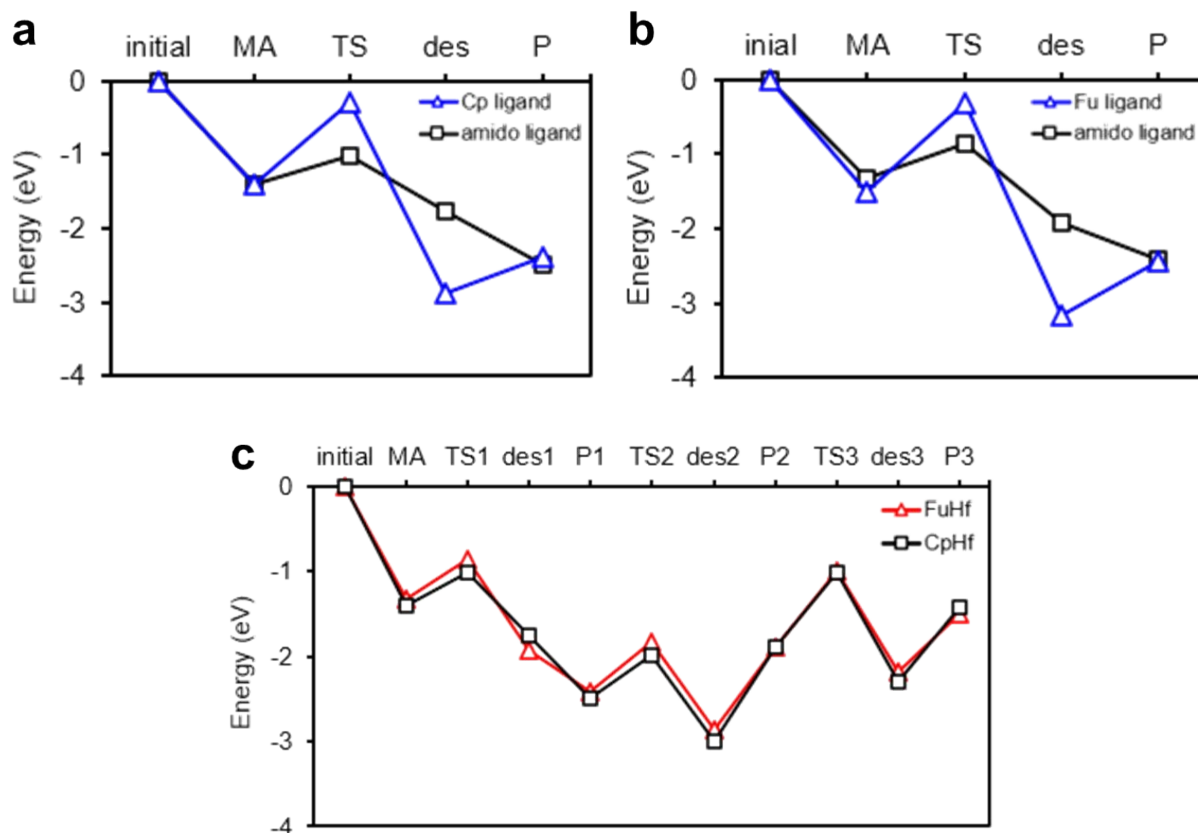

Fig. S4 Energy diagram for adsorption of precursor on the surface with the dissociation of the amido ligand or Cp-type ligand: (a) $CpHf(NMe_2)_3$, and (b) $FuHf(NMe_2)_3$. (c) Energy diagram for adsorption of $CpHf(NMe_2)_3$ and $FuHf(NMe_2)_3$ on the surface. MA = molecular adsorption of the precursor; TS*n* = transition state for the proton transfer from the surface to the *n*th ligand; des*n* = desorption of *n* byproducts; P*n* = chemisorption product after removal of *n* byproducts.

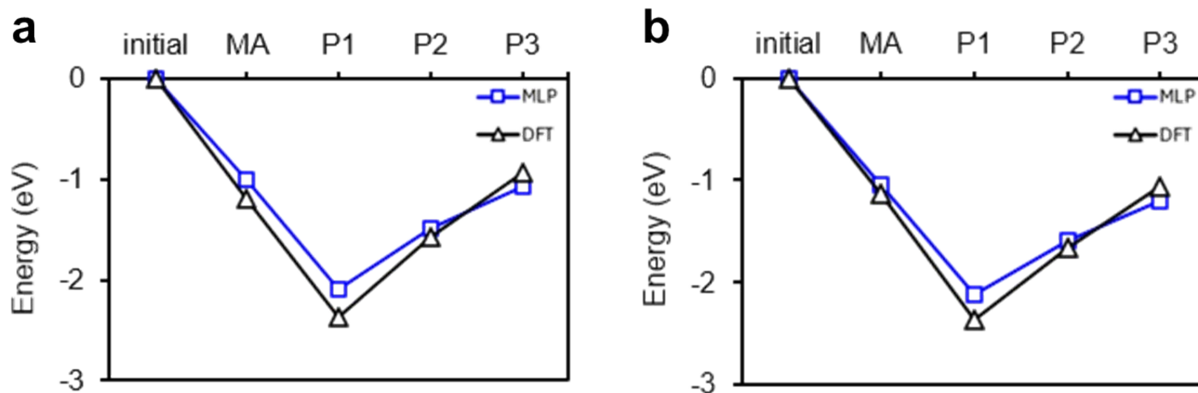

Fig. S5 Comparison of MLP and DFT calculation results for adsorption energies of precursors on hafnium oxide surface: (d) adsorption of $CpHf(NMe_2)_3$, and (e) adsorption of $FuHf(NMe_2)_3$. MA = molecular adsorption of the precursor; P*n* = chemisorption product after removal of *n* byproducts.

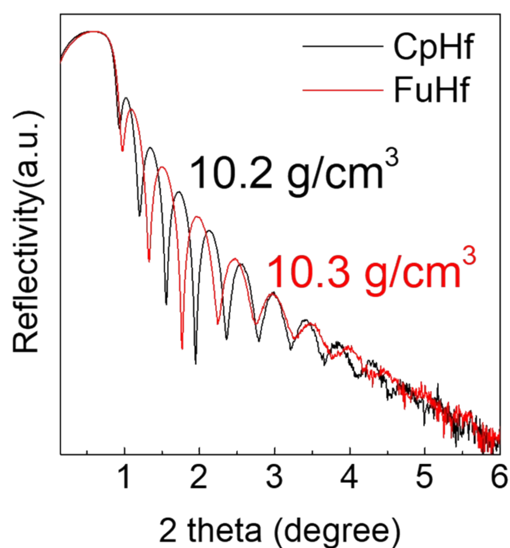

Fig. S6 XRR fitted curves for ALD HfO_2 films grown using the CpHf and FuHf precursors.

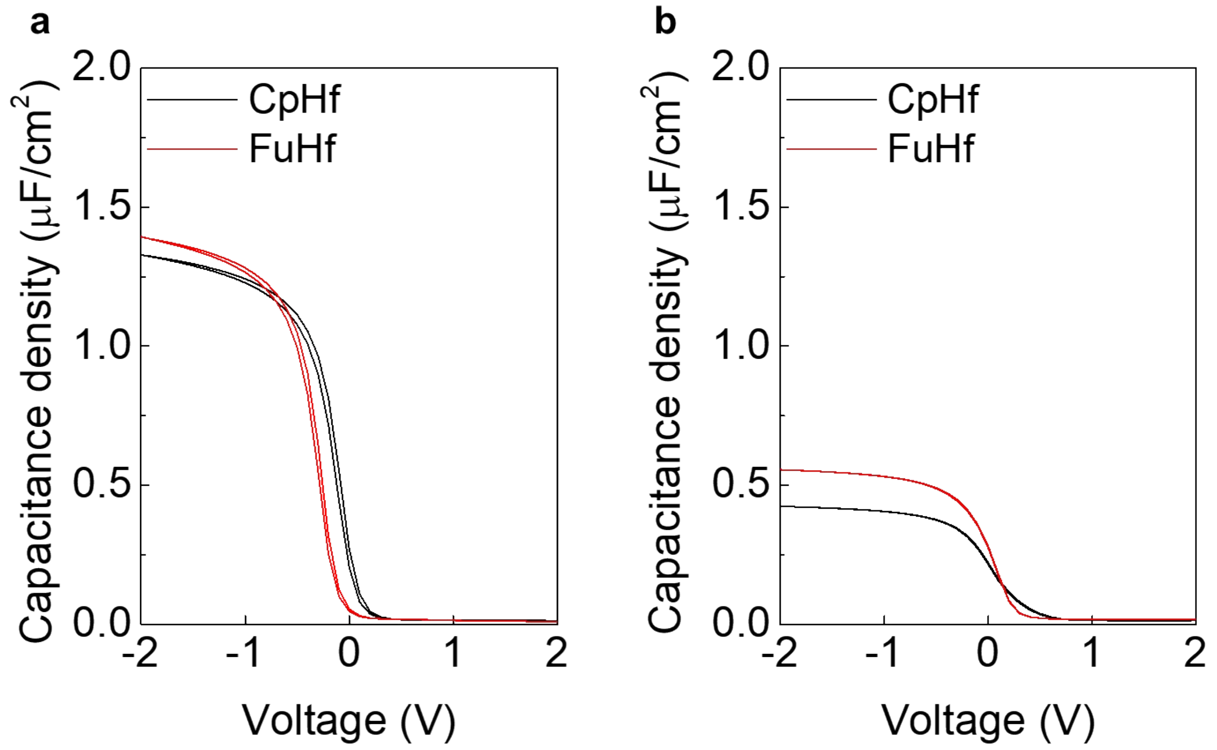

Fig. S7 Typical capacitance-voltage curves for (a) 4 and (b) 20 nm-thick HfO_2 films grown using the CpHf and FuHf precursors.