Reaction mechanism of atomic layer deposition of zirconium oxide using tris(dimethylamino)cyclopentadienyl zirconium

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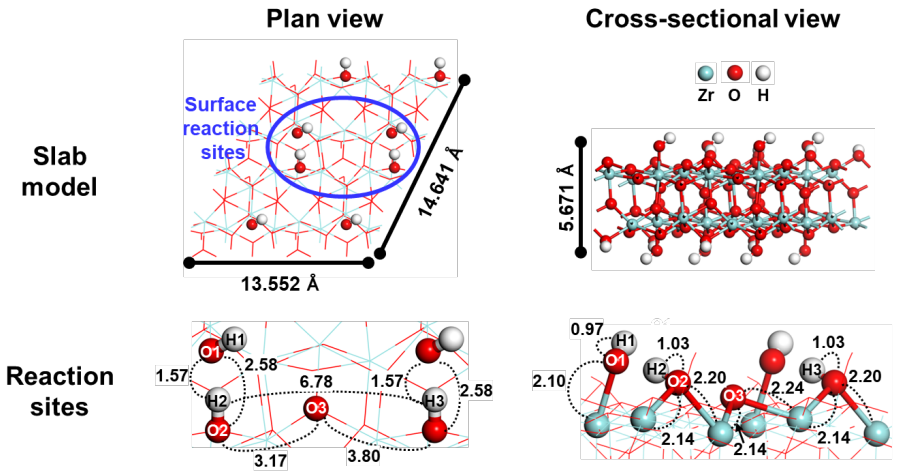
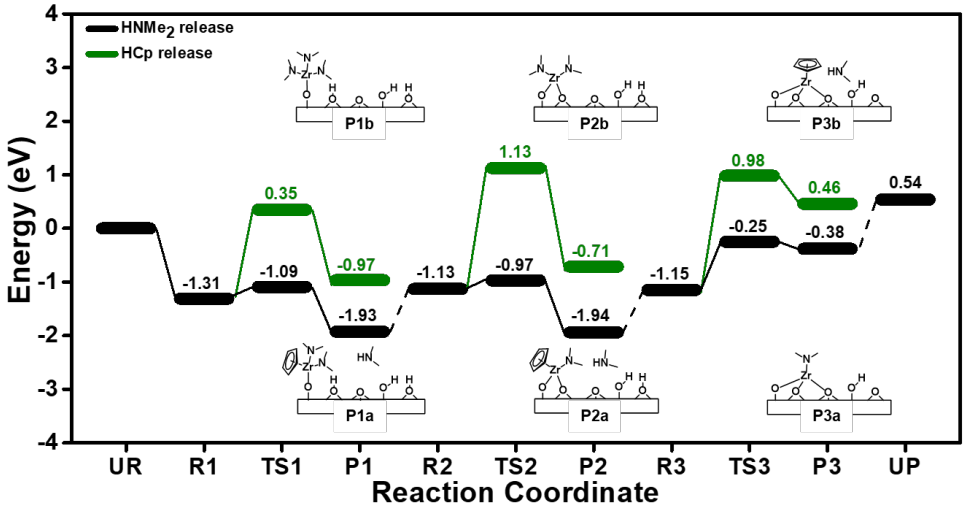
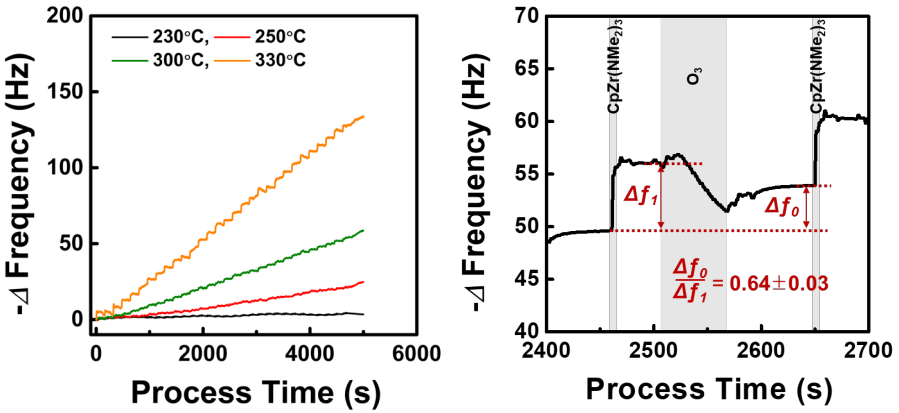
DFT calculations





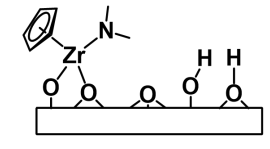
In situ QCM analysis



$$\frac{\Delta f_0}{\Delta f_1} = \frac{\mathrm{M}(ZrO_2)}{\mathrm{M}\{\mathrm{CpZr(NMe_2)_3}\} - a\mathrm{M}(\mathrm{HNMe_2}) - b\mathrm{M}(\mathrm{HC}p)}$$

Number of Cp released (x)	Number of NMe_2 released (y)	Estimated $\Delta f_0/\Delta f_1$
0	0	0.46
0	1	0.54
0	2	0.67
0	3	0.86
1	0	0.59
1	1	0.75
1	2	1
1	3	1.52

The resulting surface species



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