# Supplementary Material

## Density Functional Study on ALD precursors for Hexagonal Boron Nitride Deposition

Naoya Uene[a,b*], Takuya Mabuchi[b, c], Jin Yong[d],

Masaru Zaitsu[d], Shigeo Yasuhara[d], Takashi Tokumasu[b]

[a] *Graduate School of Engineering Tohoku University, 2-1-1, Katahira, Aoba-ku,Sendai, Japan*
[b] *Institute of Fluid Science, Tohoku University ,2-1-1, Katahira, Aoba-ku, Sendai, Japan*
[c] *Frontier Research Institute of Interdisciplinary Sciences, Tohoku University, 2-1-1, Katahira, Aoba-ku, Sendai, Japan*
[d] *Japan Advanced Chemicals Ltd., 3007-4, Kamiechi, Atsugi, Kanazawa, Japan*

*Corresponding author. E-mail: uene@nanoint.ifs.tohoku.ac.jp (Naoya Uene)

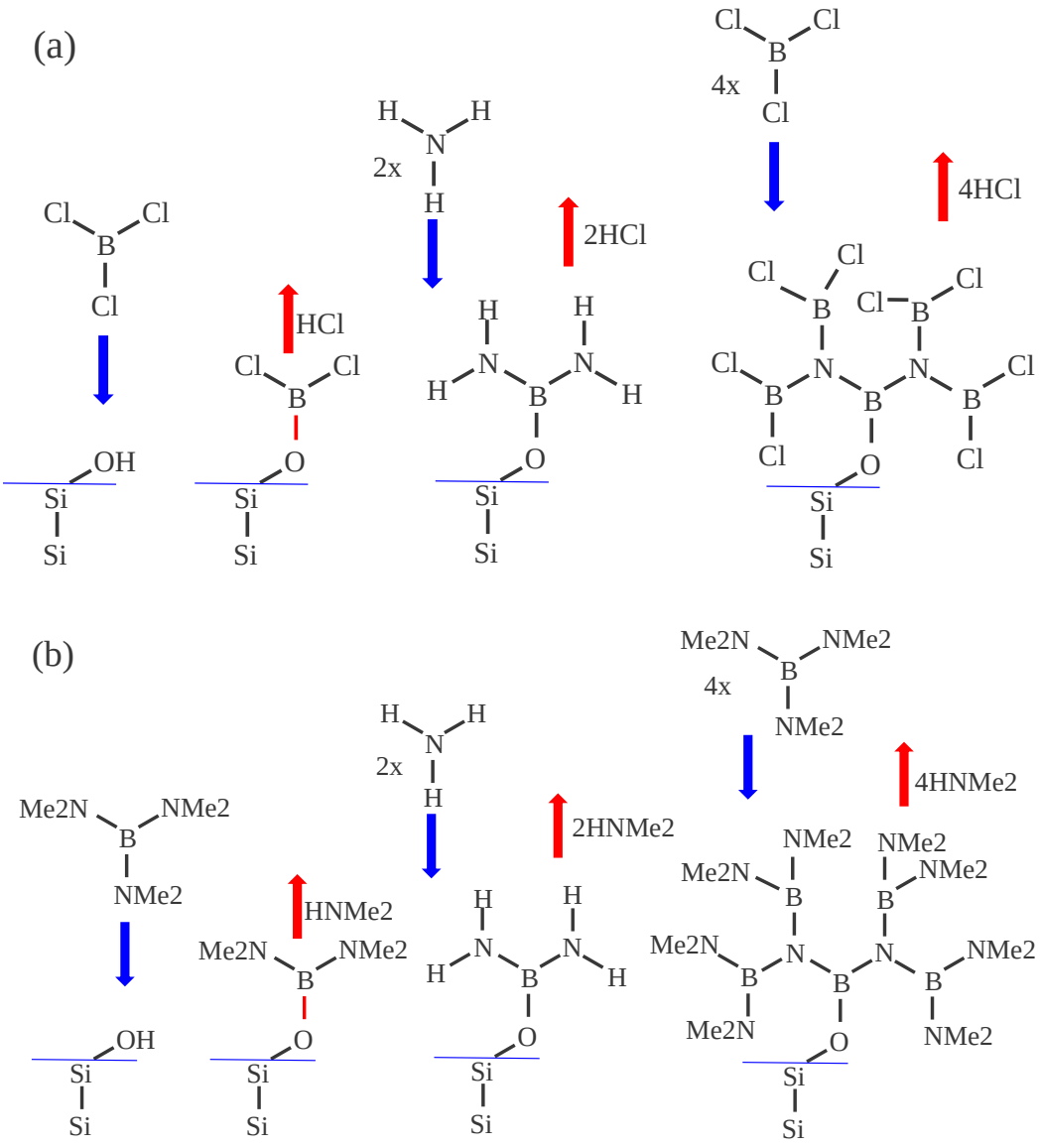


**Figure S1.** Expected ALD growth mechanisms of BN by (a) $BCl_3/NH_3$ and (b) $B(NMe_2)_3/NH_3$.