coatings

Supplementary Materials: Chemisorption and Surface Reaction of Hafnium Precursors on the Hydroxylated Si(100) Surface

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Table S1. The average bond dissociation energies (BDEs) of the hafnium precursors obtained at PBE0/6-31G(d,p) for C, H, O and def2sv for F, Cl, I and Hf level. The values in brackets are obtained by using aug-cc-pVTZ (for F and Cl) and aug-cc-pVTZ-PP (for Hf and I) basis sets.

Precursors	Average BDEs (kJ/mol)
HfI_4	359 (349)
$HfCl_4$	487 (475)
HfF_4	633 (628)
$Hf[OMe]_4$	448
$Hf[O^iPr]_4$	451
$Hf[O^tBu]_4$	454

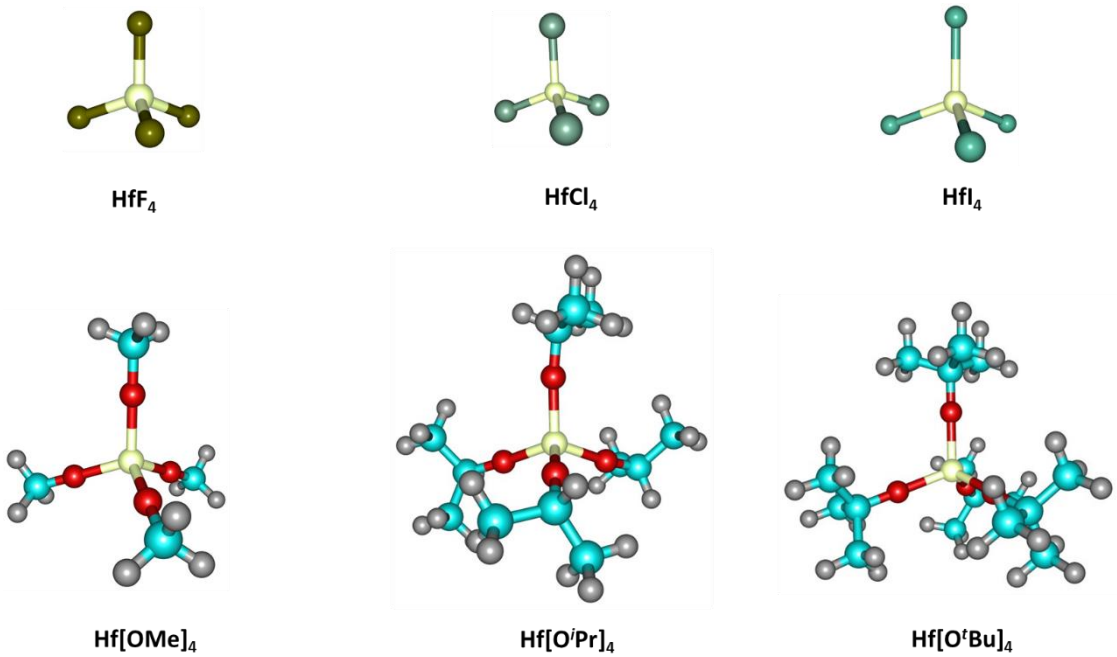

Figure S1. The optimized geometries of hafnium halides and hafnium alkoxides.