

Supplementary Material

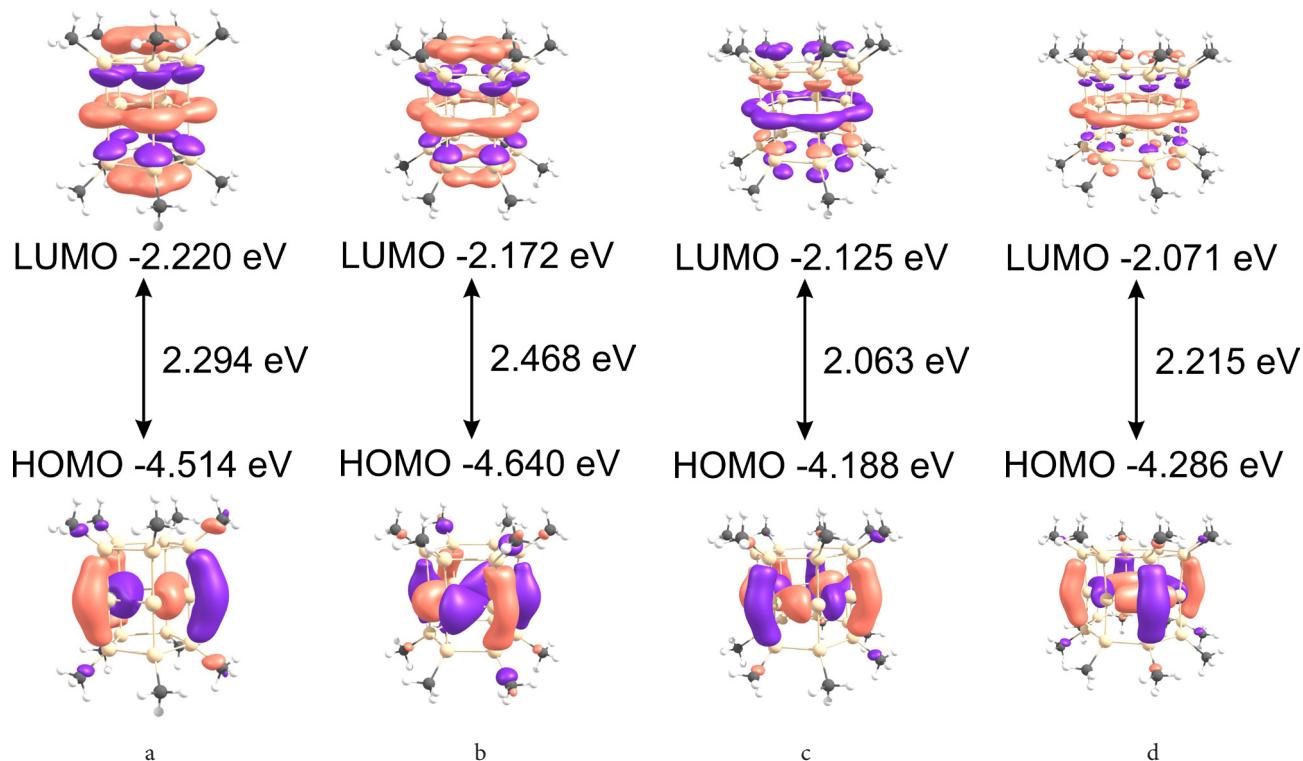


Fig. S1. (Color online) Frontier orbitals (HOMO and LUMO) of CH_3 -doped silicon biprismanes: $\text{Si}_{3n}(\text{CH}_3)_{2n}$ for $n=5$ (a), 6 (b), 7 (c), and 8 (d). HOMO and LUMO molecular orbitals are visualized using ChemCraft program package (the value of the contour envelopes is 0.03 a.u.).

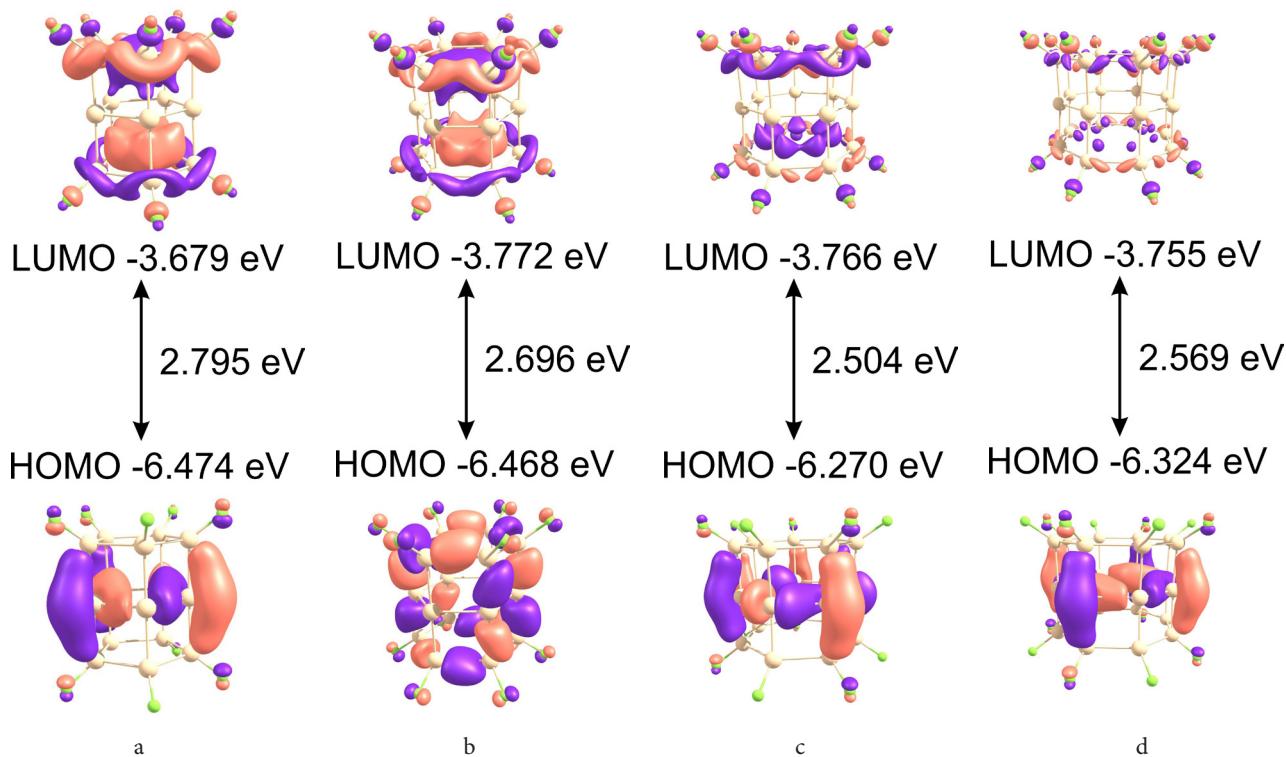


Fig. S2. (Color online) Frontier orbitals (HOMO and LUMO) of F-doped silicon biprismanes: $\text{Si}_{3n}\text{F}_{2n}$ for $n=5$ (a), 6 (b), 7 (c), and 8 (d). HOMO and LUMO molecular orbitals are visualized using ChemCraft program package (the value of the contour envelopes is 0.03 a.u.).