

Table S4. Energy (eV) for forming Si-substituted structure in different B₄C lattice sites relative to the lowest energy site over all structures. For B₁₁C^P-CBC, where inequivalent sites of each type exist, the lowest energy site of each type is listed.

Structure	Chain Center	Chain End	Equatorial	Polar
B ₁₂ -CCC	0.35	2.8	3.2	2.4
B ₁₂ -CBC	0.35	3.3	0.62	0.0
B ₁₁ C ^P -CBC	2.3	3.6	2.9	0.0