Supplemental Information

A Wide-Bandgap Graphene-like Structure C_6BN with Ultra-Low Dielectric Constant

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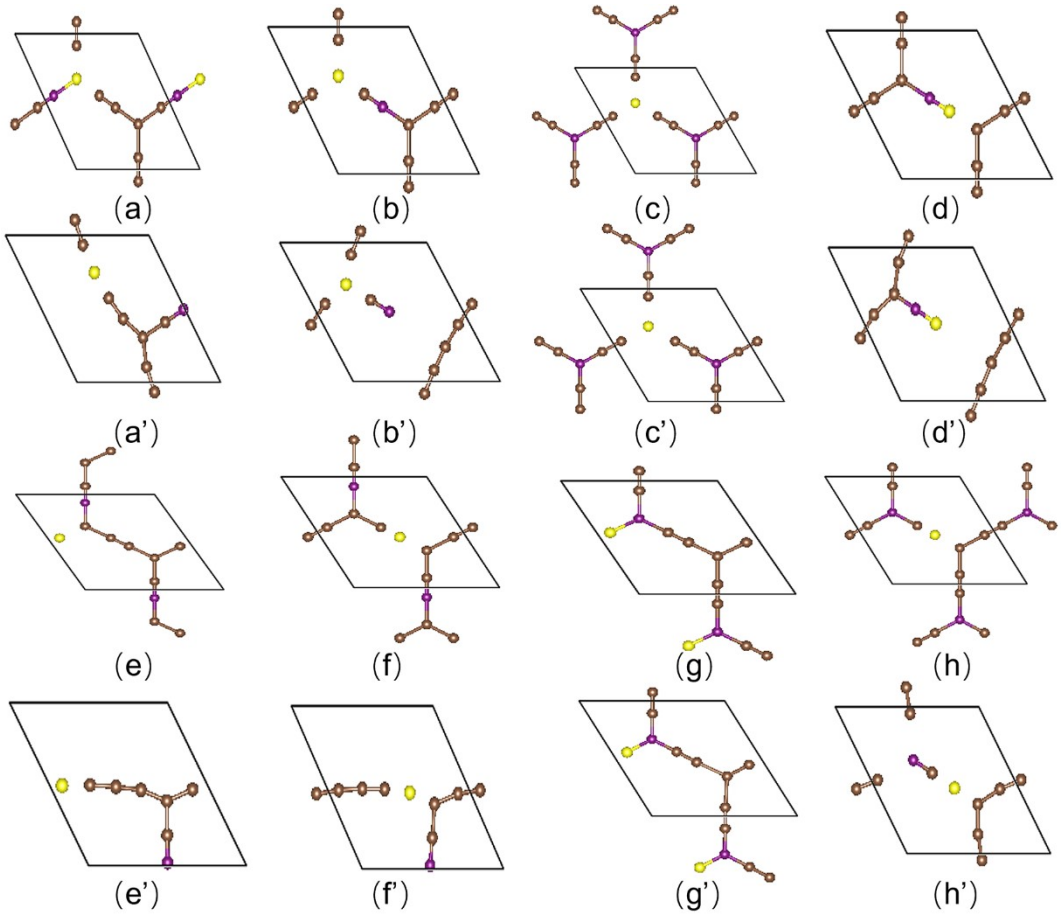

Fig. S1 Top view structure of eight models for C_6BN isomers without optimization from (a) to (h) and after optimization from (a') to (h'). The carbon, nitrogen, and boron atoms are in brown, purple, and golden yellow, respectively. The primitive cell is marked by the red box for C_6BN isomers and C_8.

Table S1 Stiffness matrixes in N/m of C_6BN.

	C_{1j}	C_{2j}	C_{3j}
C_{i1}	130.151	42.560	0
C_{i2}	42.560	130.151	0
C_{i3}	0	0	43.795

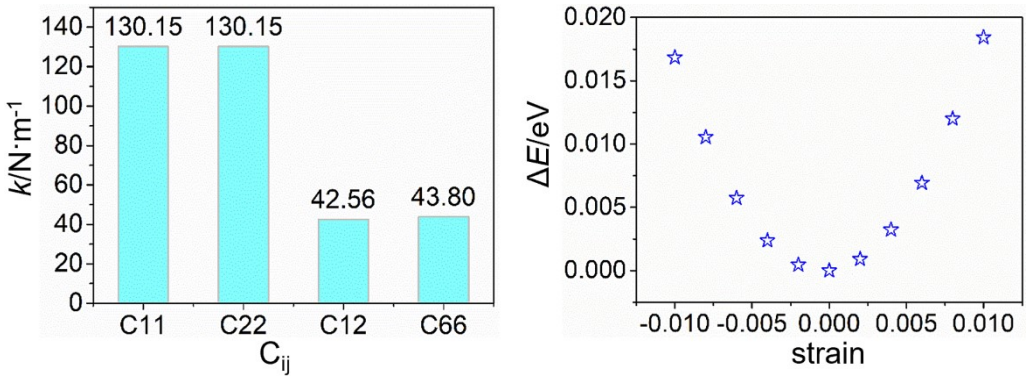

Fig. S2 Stiffness matrixes in N/m of C_6BN and the change in energy with different strain.