

Fig. S1 Schematic diagram of the doping structure for different positions of B in B₂C₃₀

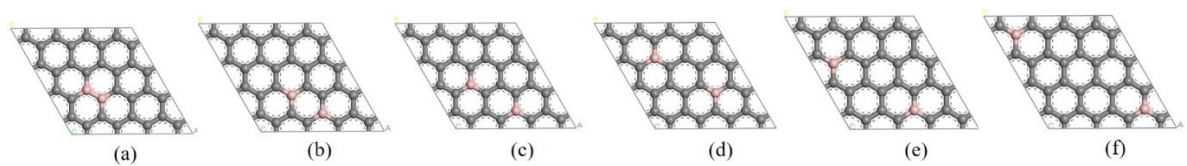


Fig. S2 Schematic diagram of the doping structure for different positions of B in B₆C₂₆

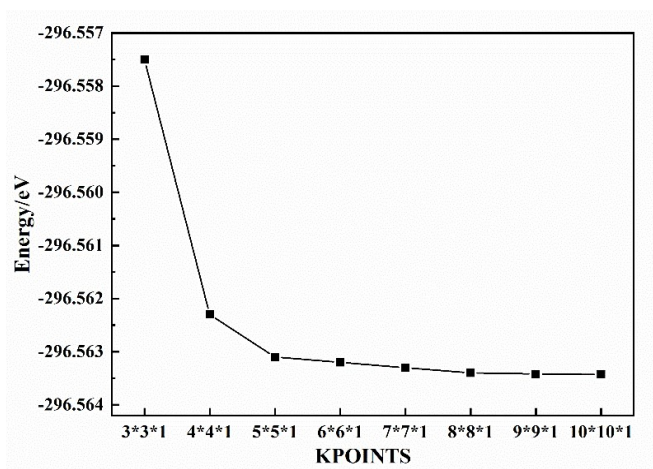


Fig. S3 The test data for K-point

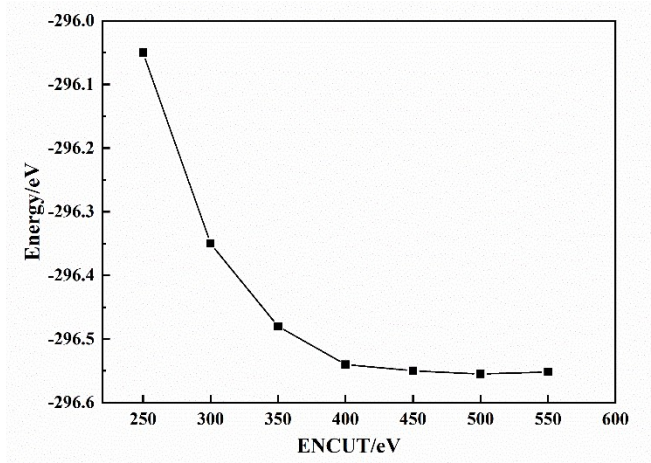


Fig. S4 The test for cut-off energy

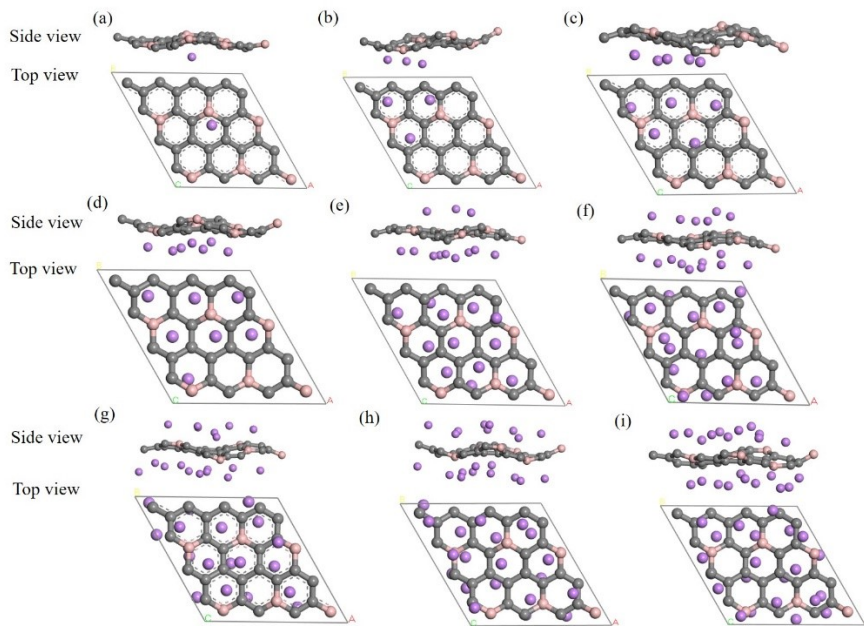


Fig. S5 Side and top views of B_6C_{26} doped structures with different amounts of Li-ion adsorption after structure optimization.

Table S1 Energy of B_2C_{30} doped structure with different positions of B

	(a)	(b)	(c)	(d)	(e)	(f)
Energy (eV)	-286.85	-287.35	-287.60	-287.41	-287.45	-287.53

Table S2 Energy of B₆C₂₆ doped structure with different positions of B

	(a)	(b)	(c)	(d)	(e)
Energy (eV)	-269.64	-269.94	-268.95	-269.46	-269.76

Table S3 The lattice constants B-doped graphene with different concentrations

System	$a=b$ (Å)
graphene	9.847
BC ₃₁	9.898
B ₂ C ₃₀	9.946
B ₆ C ₂₆	10.065
LiBC ₃₁	9.910
LiB ₂ C ₃₀	9.954
LiB ₆ C ₂₆	10.104