PCF-Graphene: A 2D sp^2 Hybridized Carbon Allotrope with a Direct Band Gap

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SUPPORTING INFORMATION

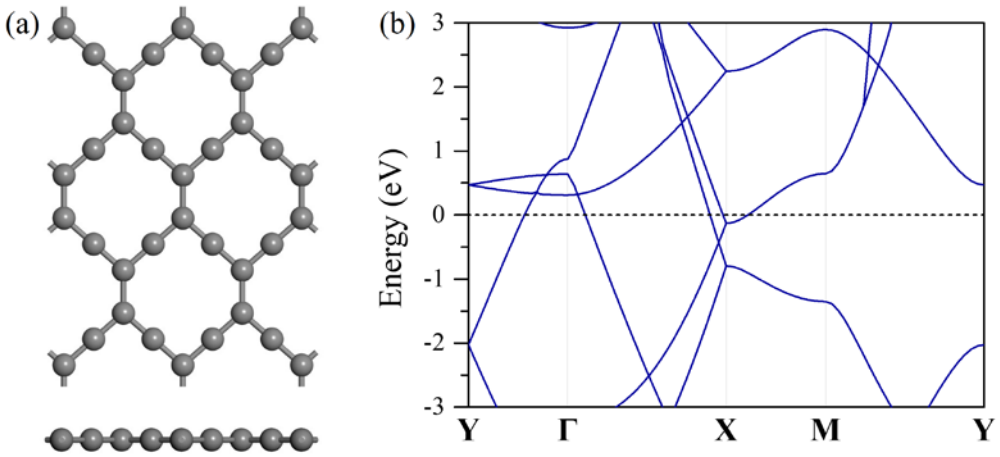

Figure S1. (a) Top and side views of the atomic configuration, and (b) electronic band structure of the planar structure originating from the exfoliated PCF-graphene.

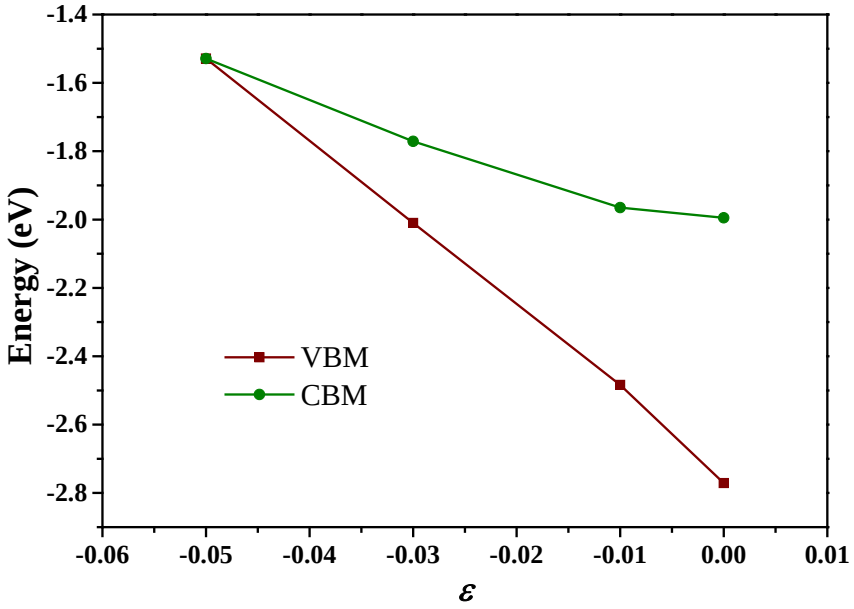

Figure S2. Energy of the VBM and CBM of PCF-graphene as a function of biaxial strain ε. The band gap is closed under a 5%-biaxial strain.

POSCAR file of optimized PCF-graphene.

PCF-graphene
1.0
4.9148001671 0.0000000000 0.0000000000
0.0000000000 5.4871001244 0.0000000000
0.0000000000 0.0000000000 25.0289001465
C
16
Direct
0.250000000 0.250000000 0.472689986
0.750000000 0.750000000 0.527310014
0.750000000 0.750000000 0.472689986
0.250000000 0.250000000 0.527310014
0.750000000 0.250000000 0.527310014
0.250000000 0.750000000 0.472689986
0.250000000 0.750000000 0.527310014
0.750000000 0.250000000 0.472689986
0.500000000 0.374410003 0.451110005
0.500000000 0.625589967 0.548889995
0.500000000 0.625589967 0.451110005
0.500000000 0.374410003 0.548889995
0.000000000 0.874410033 0.451110005
0.000000000 0.125589997 0.548889995
0.000000000 0.125589997 0.451110005
0.000000000 0.874410033 0.548889995