Supplementary Information

Graphether：A Two-Dimensional Oxocarbon as a Direct Wide-Gap Semiconductor with High Mechanical and Electrical Performances

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Table S1. Several schemes for band gap opening in graphene.

Scheme			Maximum Band Gap (eV)
spatial confinement	width ~15 nm graphene nanoribbon		0.2 (Ref. 1)
	width N=7 graphene nanoribbon		1.6 (Ref. 2)
sublattice-symmetry breaking	strain engineering	uniaxial strain	0.486 (Ref. 3)
		anisotropic biaxial strain	1.0 (Ref. 4)
		shear strain	0.4 (Ref. 4), 0.95 (Ref. 5)
	doping	B	0.14 (Refs. 6,7)
		N	0.14 (Refs. 6,7)
		O	0.50 (Ref. 7)
		P	0.67 (Ref. 8)
		S	0.57 (Ref. 8)
		Ga	0.6 (Ref. 9)
		Ge	0.4 (Ref. 9)
		As	1.3 (Ref. 9)
		Se	0.8 (Ref. 9)
	graphene antidot lattice		1.55 (Ref. 10)
surface functionalization	fully hydrogenated		3.7 (Ref. 11)
	fully fluorinated		3.48 (Ref. 12)
	half hydrogenated		0.43 (Ref. 12)
	half hydrogenated and half fluorinated		3.70 (Ref. 12)
	fully oxidized		4.0 (Ref. 13)
heterostructure	graphene/h-BN		0.053 (Ref. 14), 0.16 (Ref. 15)
	graphene/SiC		0.26 (Ref. 16)
	graphene/fully hydroxylated SiO_2		0.023 (Ref. 17)
	graphene/O-terminated SiO_2		0.044 (Ref. 17)
electrically tunable band gap in multilayer graphene	bilayer		0.1 (Ref. 18), 0.25 (Ref. 19)
	trilayer		0.12 (Ref. 20)

Computational details of the carrier mobility and in-plane stiffness

We estimate the carrier mobility for graphether at room temperature (300 K) by using the equation $\mu_x \approx \frac{e\hbar^3\left(\frac{5C_x+3C_y}{8}\right)}{k_B T m_x^{\frac{3}{2}} m_y^{\frac{1}{2}}\left(\frac{9E_{1x}^{\ 2}+7E_{1x}E_{1y}+4E_{1y}^{\ 2}}{20}\right)}$, where m_x is the effective mass in the transport direction and m_y is the effective mass in another direction. The term E_1 defined by $E_1 = \frac{\Delta V}{(\Delta l / l_0)}$ represents the DP constant of the valence-band minimum (VBM) for hole or the conduction-band maximum (CBM) for electron along the transport direction. Here, ΔV denotes the energy change of VBM or CBM when graphether is compressed or dilated from the equilibrium l_0 by a distance of Δl. The term C_x (C_y) is the in-plane stiffness of the longitudinal strain in the x (y) direction, which can be derived from $\frac{\Delta E}{S_0} = C_x \frac{(\Delta l / l_0)^2}{2}$. ΔE denotes the total energy difference under each strain, and S_0 is the lattice area of pristine graphether. We use $\Delta l/l_0$ ranging from -0.5% to 0.5% to fit the values of C_{2D} and E_1 (Fig. S1).

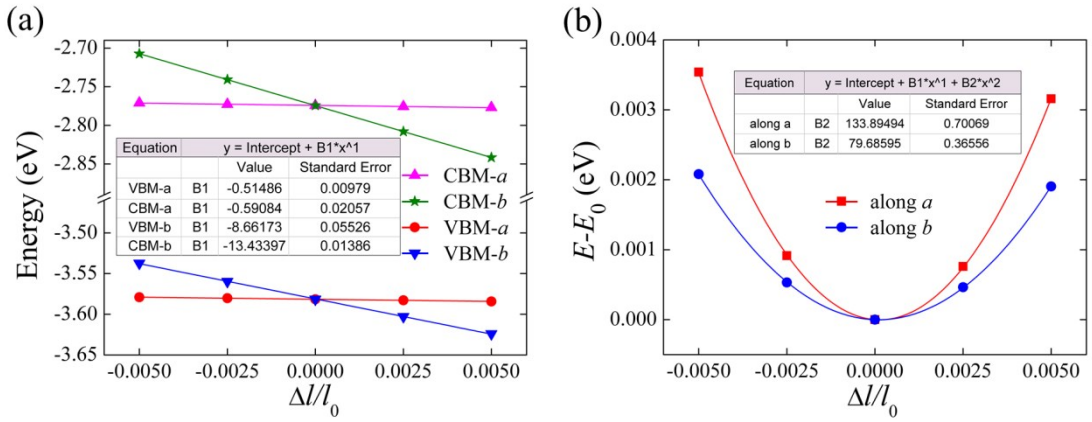

Fig. S1 (a) DP constants and (b) in-plane stiffness of graphether along x and y directions at the HSE06 level of theory.

Table S2. Lattice parameter, interlayer distance (d_z), binding energy (E_b), and band gap for bilayer graphether.

stacking pattern	lattice parameters (Å)		d_z (Å)	E_b (meV Å^{-2})	band gap (eV)
	a	*b*			
monolayer	7.229	5.155	-	-	2.39
AA	7.233	5.152	2.003	-33.44	2.27
AB	7.227	5.154	3.451	-9.42	2.31
AC	7.233	5.150	2.150	-27.75	2.27
AD	7.227	5.154	3.516	-9.12	2.32

Table S3. Structural informations of monolayer graphether and *Pmn*2$_1$-BNO.

Structure	Space Group	Lattice Parameters	Wyckoff Positions (fractional)			
			atoms	*x*	*y*	*z*
Graphether	*Pmmn*	a=3.6144 Å	C(4f)	0.2881	0	0.5180
		b=2.5775 Å	O(2a)	0	0	0.5570
		c=25.0000 Å				
		α=β=γ=90°				
*Pmn*2$_1$-BNO	*Pmn*2$_1$	a=2.6493 Å	B(2a)	0	0.4811	0.7062
		b=25.0000 Å	N(2a)	0	0.4825	0.2816
		c=3.6579 Å	O(2a)	0	0.4414	0.9897
		α=β=γ=90°				

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