Electronic Supplementary Information (ESI)

The origin of instinct charge transport for Dirac carbon sheet materials: Roles of acetylenic linkage and electron-phonon couplings

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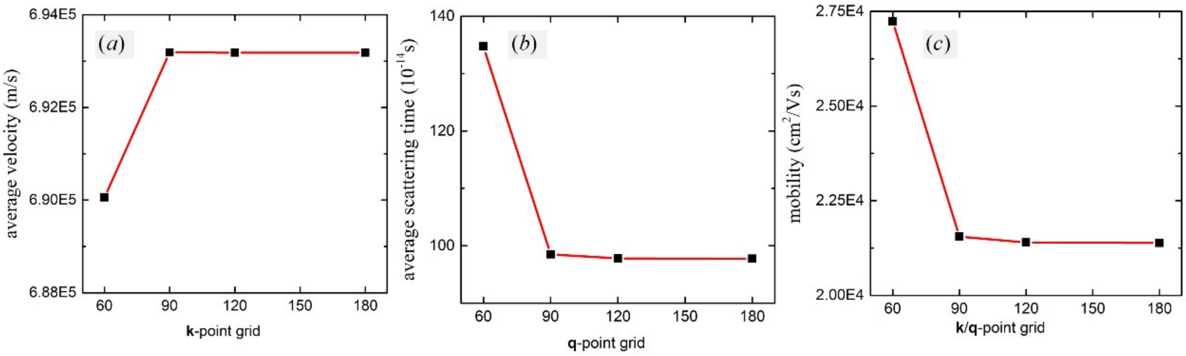

Fig. S1 Electron average velocity (a), average scattering time (b) and mobility (c) computed with respect to varying density of **k**/**q**-point grids.

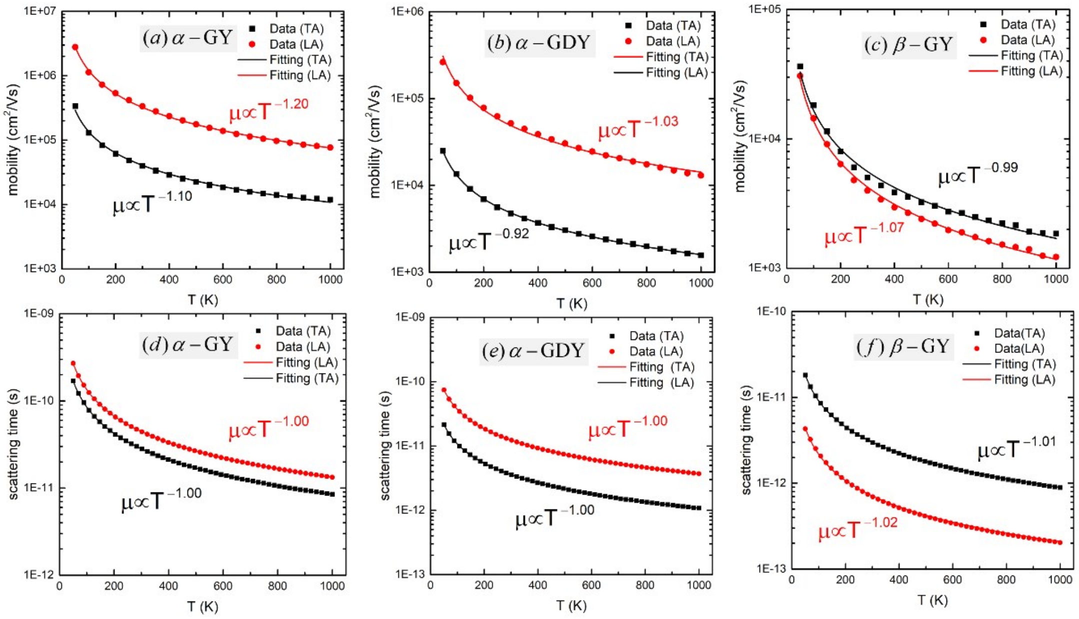

Fig. S2 Electron mobility (a-c) and scattering time at Dirac point (d-f) of TA/LA together with the fitting line for α-GY, α-GDY and β-GY, respectively.

Table S1 Character table of reducible representation and E_{2g} irreducible representation for these Dirac materials.

D_{6h}	E	$2C_6$	$2C_3$	C_2	$3C_2^{'}$	$3C_2^{''}$	i	$2S_3$	$2S_6$	σ_h	$3\sigma_d$	$3\sigma_v$
$\Gamma_{N(1)}$	3m	0	0	0	(2-m)/3-2	0	0	-4	0	m	0	(m-2)/3+2
$\Gamma_{N(2)}$	3m	0	0	0	0	-2	0	0	0	m	2	0
E_{2g}	2	-1	-1	2	0	0	2	-1	-1	2	0	0

Where $\Gamma_{N(1)}$, $\Gamma_{N(2)}$ are the reducible representation for structure with uniform acetylenic linkages (i.e., graphene, *α*-GY, *α*-GDY) and un-uniform acetylenic linkages (i.e., *β*-GY), respectively. m is the total number of atom, satisfying $m=2n+2$ for uniform acetylenic linkages and $m=2n+6$ for un-uniform acetylenic linkages, where n is the number of acetylenic linkages. It is easy to use equation

$$N_\alpha = \frac{1}{g}\sum_G C_G \chi(G)\chi^*(G) \qquad \text{(S1)}$$

which shows how many times a given irreducible representation α is contained in a reducible one. Therefore, we can obtain the number of E_{2g} modes $N(E_{2g}) = \frac{1}{3}(2n+3)$ for graphene, *α*-GY, *α*-GDY and $N(E_{2g}) = \frac{1}{3}(2n+6)$ for *β*-GY.

Lattice Vibration and Charge Transport

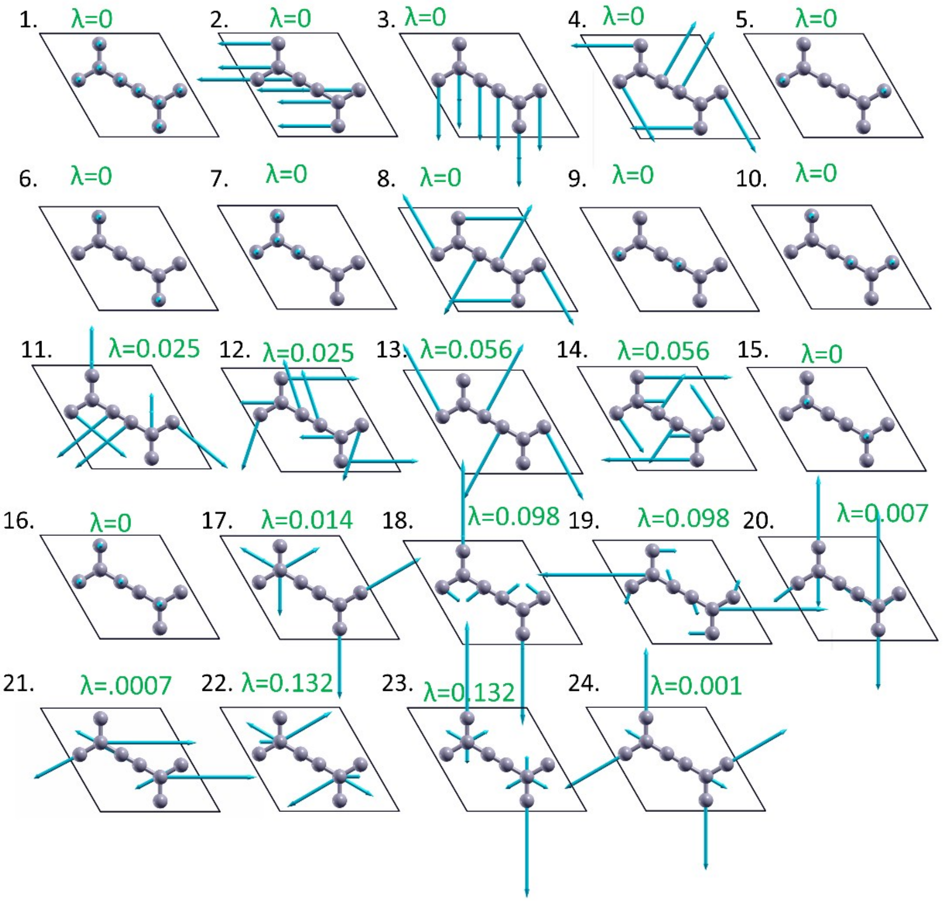

Fig. S3 The vibrational direction and amplitude of all the phonon modes at **Γ** together with EPC strength for α-GY. The strength of ZA/TA/LA phonon modes are forced to set to zero due to acoustic sum rule.

The vibration of the 3 acoustic phonon and 21 optical phonon at **Γ** are shown in Fig. S1. Apparently, vibration along the chemical bond direction tends to cause a large EPC strength and vibration perpendicular to the bond leads to a small EPC strength. In particular, phonon vibration out-of-plane will have no interaction with electron and get λ=0, which is agreeing well with our group analysis.

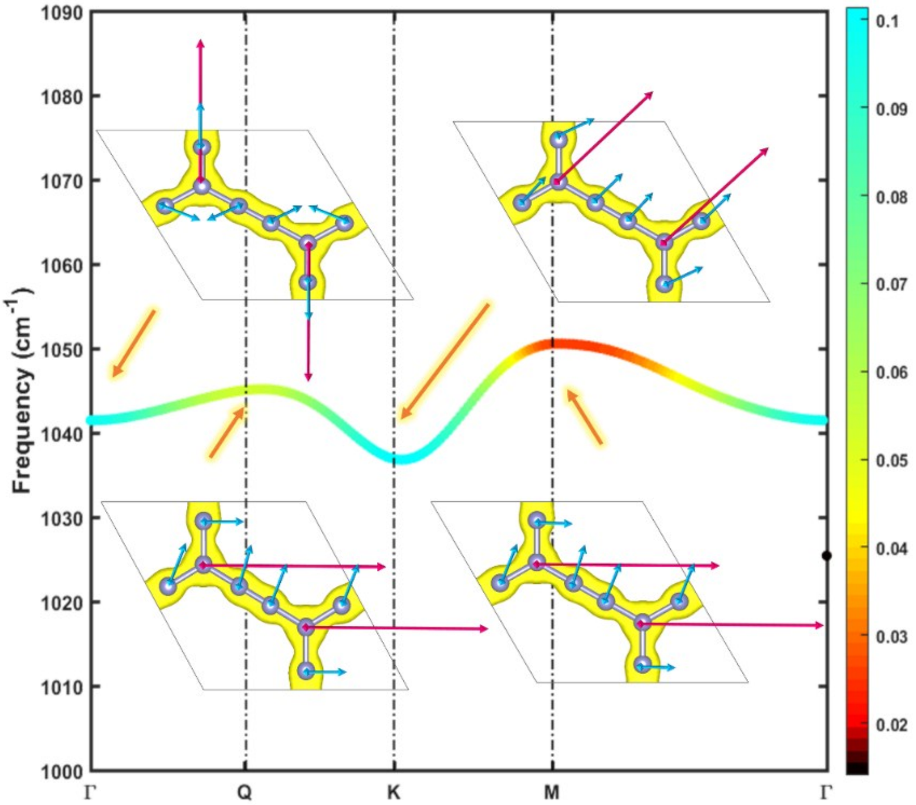

Fig. S4 The vibration of $^{2}E_{2g}^{L}$ mode together with the charge density at different **q** points along **Γ-K-M-Γ** for α-GY.

As shown in Fig. S2, at the high symmetry point **Γ** and **K**, the phonon vibrates along the direction of the chemical bond (red arrow), indicating that the vibrations are easier to destroy the overlap of π orbital and damage charge transport channel, and we find a large EPC strength (~0.1), as expected. Conversely, at the **Q** and **M**, the phonon vibrates at an angle to the chemical bond direction (red arrow), implying the overlap of π orbital is weakly destroyed. Indeed, the corresponding EPC is relatively small.

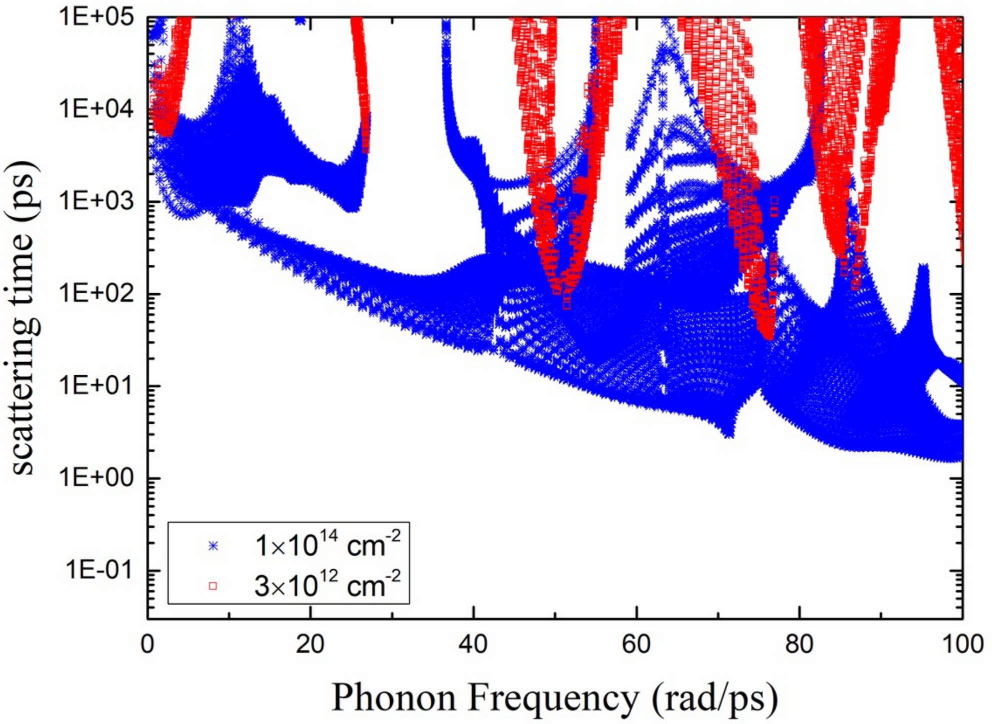

Fig. S5 Phonon scattering time from EPC at different carrier connections for *α*-GY at room temperature.