Supporting Information

Porous carbon-based metal-free monolayers towards to high stable and flexible wearable thermoelectric and microelectronics

Xiaoran Shi[1], Hongsheng Liu[1], Ziyu Hu[2*], Jijun Zhao[1,3], Junfeng Gao[1,3*]

[1]*Key Laboratory of Materials Modification by Laser, Ion and Electron Beams (Dalian University of Technology), Ministry of Education, Dalian 116024, China*

[2]*College of Mathematics and Physics, Beijing University of Chemical Technology, Beijing 100029, People's Republic of China*

[3]*State Key Laboratory of Structural Analysis for Industrial Equipment, Dalian University of Technology, Dalian, 116024, China*

Corresponding authors: gaojf@dlut.edu.cn and huziyu@mail.buct.edu.cn

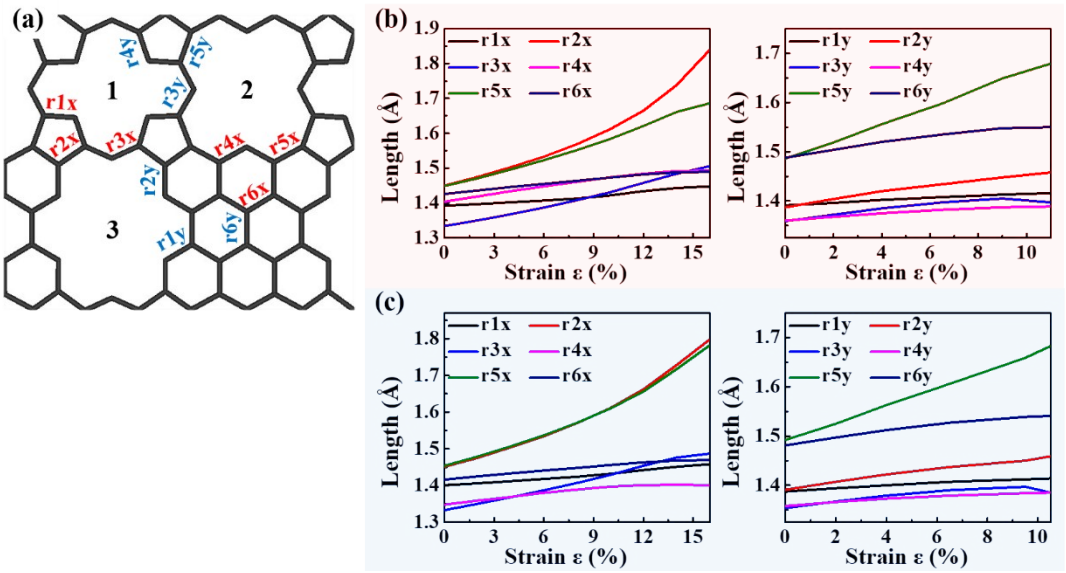

Fig. S1 (a) Schematic illustrations of the bonds of g-MC-A and g-MC-B. Strain-length curves for (b) g-MC-A and (c) g-MC-B along x/y direction.

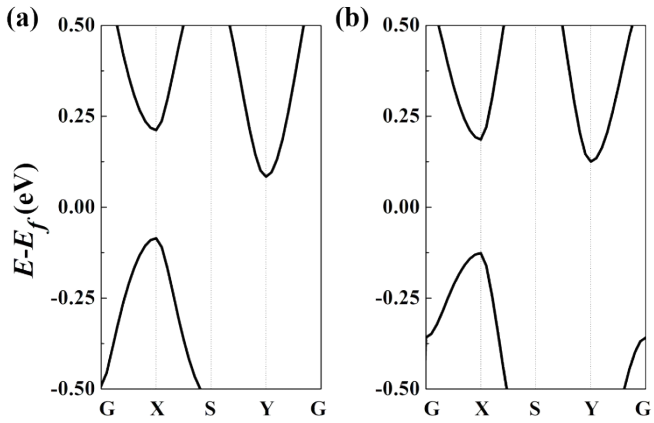

Fig. S2. Band structures of (a) g-MC-A and (b) g-MC-B on the HSE06 level, the fermi level is shifted to zero.

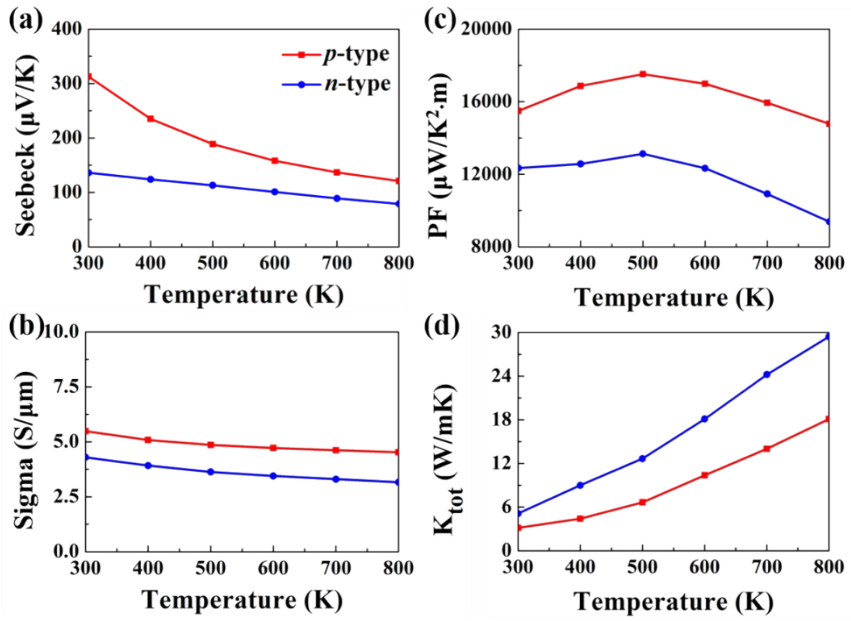

Fig. S3 Thermoelectric parameters of g-MC-A. (a) Seebeck coefficient. (b) Conductivity. (c) Power factor. (d) Thermal conductivity.

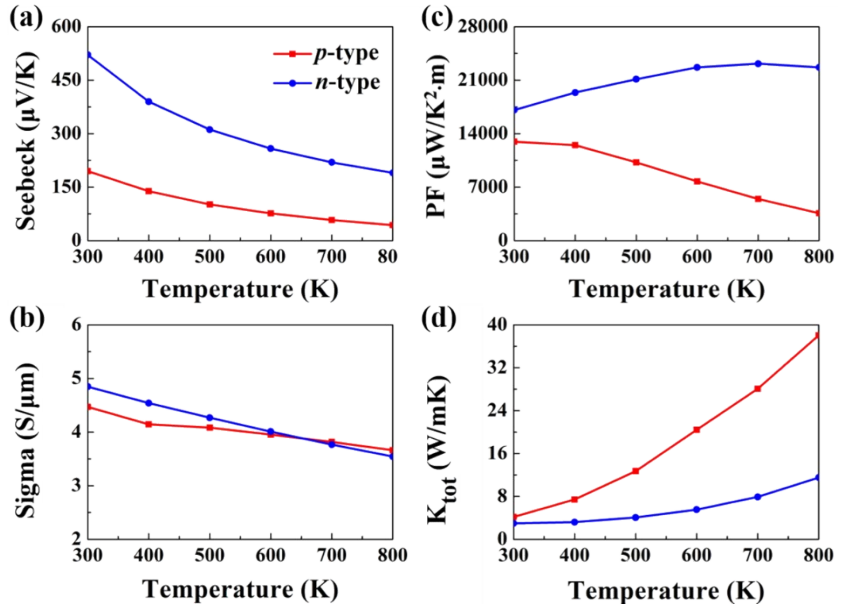

Fig. S4 Thermoelectric parameters of g-MC-B. (a) Seebeck coefficient. (b) Conductivity. (c) Power factor. (d) Thermal conductivity.

Table S1 2D elastic modulus, effective masses, deformation potential and carrier mobilities. The orientations of x and y are defined in Fig. 1.

Material	Carrier	C_{2D} (N/m)	m^* (m_0)	E_1 (eV)	μ ($10^3 cm^2V^{-1}s^{-1}$)
g-MC-A	electron-x	155	0.23	1.58	25.7
	electron-y	153	0.20	4.77	3.9
	hole-x	155	0.07	3.34	49.2
	hole-y	153	0.48	3.07	1.6
g-MC-B	electron-x	154	0.32	1.67	11.4
	electron-y	155	0.16	5.13	5.0
	hole-x	154	0.25	3.28	5.0
	hole-y	155	0.33	3.35	2.8

Table S2 The relaxation time τ for g-MC.

Material	Carrier	τ (ps)
g-MC-A	electron-x	3.36
	electron-y	0.43
	hole-x	1.96
	hole-y	0.44
g-MC-B	electron-x	2.07
	electron-y	0.45
	hole-x	0.71
	hole-y	0.53