Supporting Information for:

Tunable bending modulus and bending limit of oxidized graphene

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1. Bending models of random GO

The random GO models with epoxide and hydroxyl groups randomly distributed are generated by the Monte Carlo method. For each coverage and hydroxyl-to-epoxide ratio, we first generate ten initial structures and then optimize them to find the most stable one with the lowest total energy for further bending study. Following this rule, we obtain two random GO models ($C_{168}H_4O_{44}$) with the same coverage of 50% and the same hydroxyl-to-epoxide ratio of 1:10. The optimized random GO models and their bent nanotube counterparts are presented in Fig. S1. It can be noticed that wrinkles and ether groups are existed in the random GO. Moreover, bending can further transform the epoxide into ether.

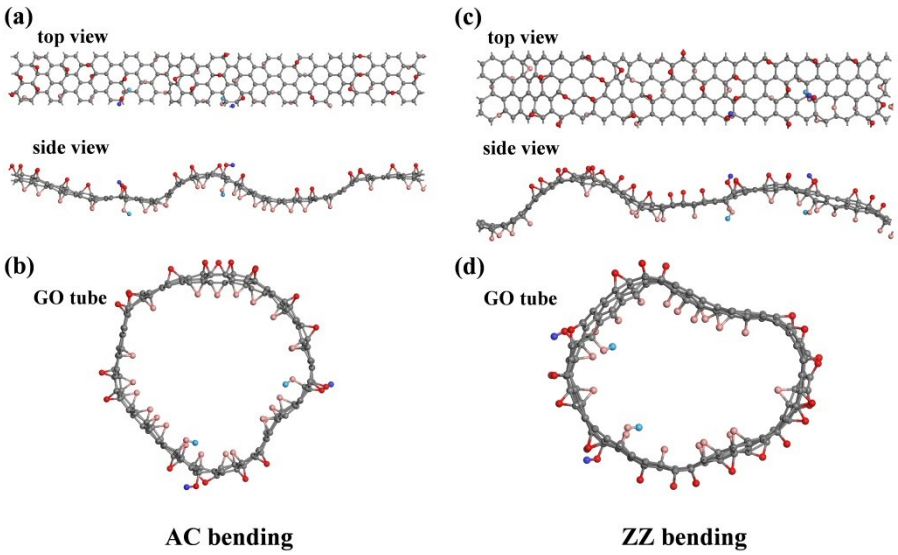

Fig. S1 Optimized structures for the random GO models: (a) top and side view of flat GO and (b) its nanotube counterpart under AC bending; (c) top and side view of flat GO and (d) its nanotube counterpart under ZZ bending. The carbon, oxygen and hydrogen atoms are displayed in gray, red and blue separately. The functional groups lying in two sides of the graphene basal plane are marked with different color depths.

2. Comparison of bending modulus

We use the lattice parameter in bending direction as the circumference to determine the curvature of bent random GO. The calculated bending modulus D of random GO is listed in Table S1, along with those of ordered GO for comparison.

Table S1 Comparison of the bending modulus D between the ordered and random GO models where the OH:O is the hydroxyl-to-epoxide ratio.

	AC bending		ZZ bending	
Parameters	ordered GO	random GO	ordered GO	random GO
Coverage	50%	50%	50%	50%
OH:O	2:1	1:10	2:1	1:10
κ (nm^{-1})	0.918	1.077	2.016	1.274
D (nN·nm)	0.64	0.41	0.67	0.17