Electronic Supplementary Information

Super flexibility and Stability of Graphene Nanoribbons under Severe Twist

Authors: D. Xia[ab], Q. Li[b], Q.Z. Xue[c], C.Y. Liang[a*] and M.D. Dong[b*]

[a]Research Institute for Energy Equipment Materials, Tianjin Key Laboratory of Materials Laminating Fabrication and Interface Control Technology, Hebei University of Technology, Tianjin 300130, China
[b]Interdisciplinary Nanoscience Center (iNANO), Aarhus University, Aarhus 8000, Denmark,
[c]State Key Laboratory of Heavy Oil Processing; College of Science, China University of Petroleum, Qingdao 266580, Shandong, China
* Address correspondence to liangchunyong@126.com; dong@inano.au.dk (M.D.)

Table S1. h value used in different methods

Authors	Year	Potential/Method	h (Å)
Zhang et al.[1]	2013	NEMD (COMPASS)	3.35
Zheng et al.[2]	2013	MD (COMPASS)	3.40
Jing et al.[3]	2012	MD (COMPASS)	3.40
Zheng et al.[4]	2010	MD (COMPASS)	3.40
Zhong et al.[5]	2011	MD (Tersoff-Brenner)	3.35
Liu et al.[6]	2007	Ab initio	3.34
Van Lier et al.[7]	2000	Ab initio	3.40
Sakhaee-Pour et al.[8]	2009	Atomistic Modeling	3.40
Reddy et al.[9]	2006	Tersoff-Brenner	3.40
Zhang et al.[10]	2012	DFT	3.34
Lee et al.[11]	2008	Numerical Simulations	3.35

Table S2. The energy components (kcal/mol) of the GNR under different twist angle

dθ	E_{bond}	E_{angle}	$E_{torsion}$	E_{oop}	$E_{bond-bond}$	$E_{bond-angle}$	$E_{end\ bond-torsion}$	$E_{middle\ bond-torsion}$	$E_{angle-torsion}$	$E_{angle-angle\ torsion}$	$E_{bond-bond-1-3}$	E_{VDW}	$E_{electrostatic}$
0°	907.6	620.3	76441.3	130.0	6.6	-51.3	-1095.1	94.0	383.3	-2.8	35.4	1818.5	212.1
30°	946.8	663.0	76457.2	130.1	6.7	-51.8	-1154.4	105.3	379.0	-3.4	36.3	1833.9	213.1
60°	915.6	649.8	76436.1	127.8	2.1	-47.0	-1051.7	90.7	380.6	-4.0	36.0	1799.8	213.5
90°	928.2	663.8	76447.1	125.7	-6.1	-37.3	-1001.7	78.9	380.8	-2.2	28.0	1791.5	216.5
120°	923.7	754.9	76457.3	132.8	-5.9	-29.7	-921.3	70.9	370.8	-3.2	21.1	1772.8	213.7
150°	947.4	807.5	75769.0	120.9	-20.5	-4.2	-712.8	39.6	363.8	-2.9	20.8	1722.0	225.6
180°	1018.0	982.4	76444.0	123.8	-22.1	22.6	-618.6	14.8	360.9	-2.7	15.0	1707.9	176.0
210°	1059.6	1173.7	76481.0	164.8	-23.5	49.0	-422.6	-10.0	343.1	-2.2	18.6	1688.0	152.6
240°	998.5	1201.5	76593.0	423.9	-31.9	45.7	-261.6	-45.6	290.2	-0.5	4.0	1481.5	159.7

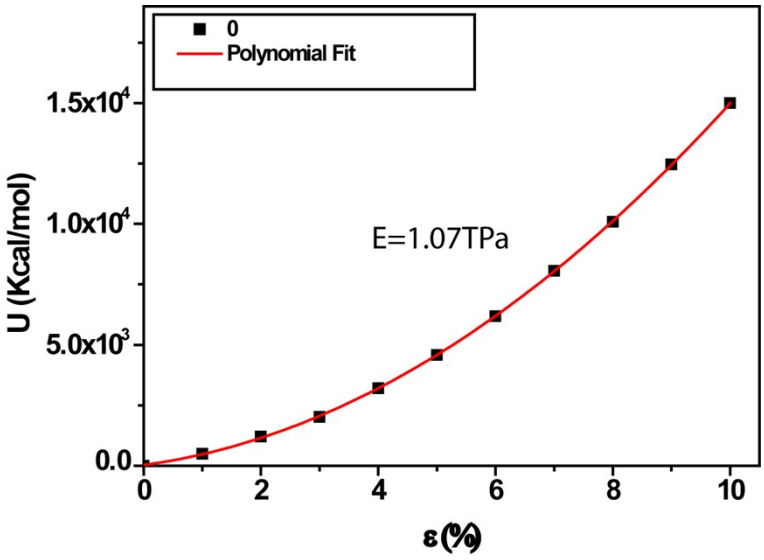

Fig. S1. U-ε curve of armchair graphene (the red line represents polynomial fitting).

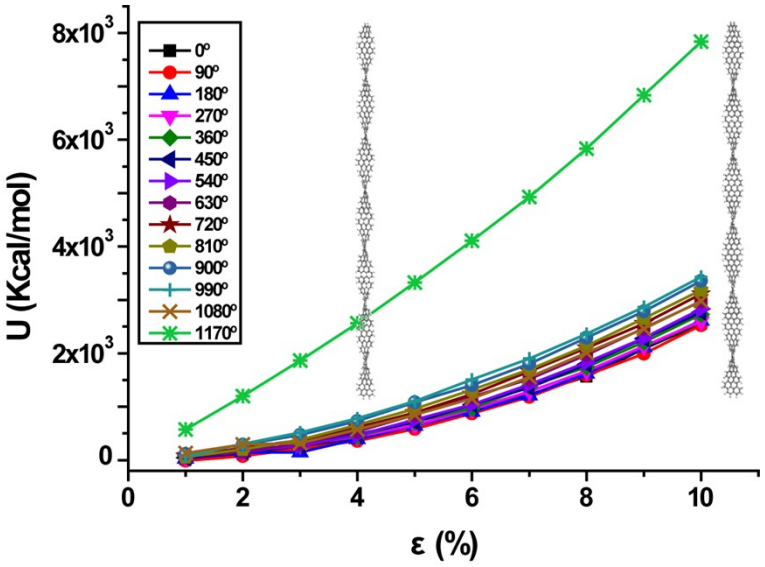

Fig. S2. U-ε curves of armchair graphene under extreme tensile displacement. The insets are the snapshots of graphene twisted by 990º and 1170º rotations, respectively.

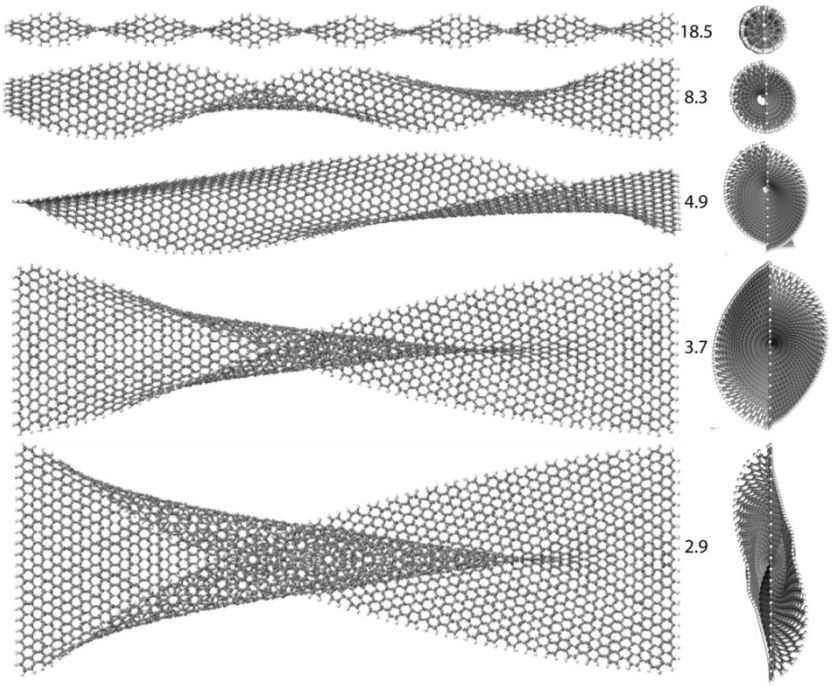

Fig. S3. Snapshots of the twist graphene with different aspect ratios under overloaded rotations (left panel: side view; right panel: top view).

1. K. S. Novoselov, A. K. Geim, S. Morozov, D. Jiang, Y. Zhang, S. a. Dubonos, I. Grigorieva and A. Firsov, *science*, 2004, **306**, 666-669.
2. A. A. Balandin, S. Ghosh, W. Bao, I. Calizo, D. Teweldebrhan, F. Miao and C. N. Lau, *Nano Lett.*, 2008, **8**, 902-907.
3. R. Nair, P. Blake, A. Grigorenko, K. Novoselov, T. Booth, T. Stauber, N. Peres and A. Geim, *Science*, 2008, **320**, 1308-1308.
4. Q. Zheng, Y. Geng, S. Wang, Z. Li and J.-K. Kim, *Carbon*, 2010, **48**, 4315-4322.
5. K. Wakabayashi, *Phys. Rev. B*, 2001, **64**, 125428.
6. V. Barone, O. Hod and G. E. Scuseria, *Nano Lett.*, 2006, **6**, 2748-2754.
7. Y.-W. Son, M. L. Cohen and S. G. Louie, *Nature*, 2006, **444**, 347-349.
8. A. Sakhaee-Pour, *Solid State Communications*, 2009, **149**, 91-95.
9. C. Reddy, S. Rajendran and K. Liew, *Nanotechnology*, 2006, **17**, 864.
10. J. Zhang, J. Zhao and J. Lu, *Acs Nano*, 2012, **6**, 2704-2711.
11. C. Lee, X. Wei, J. W. Kysar and J. Hone, *Science*, 2008, **321**, 385-388.