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Tunable in-plane torsional strength of surface functionalized two dimensional nanomaterials

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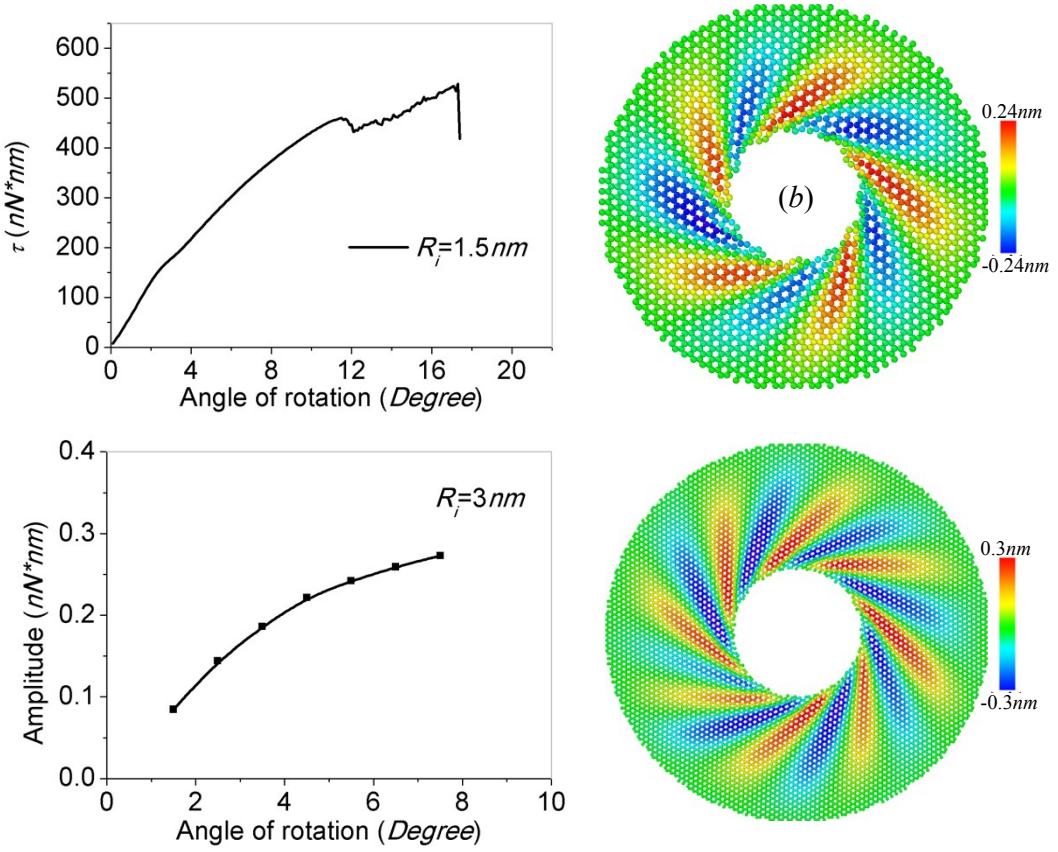

Fig. S1 Mechanical characteristics of circular graphene annulus subjected to in-plane rotation at inner edge. (***a***) Atomistic model of circular under circular rotation at inner edge. The slave domain represents the inner and outer boundaries which are not plotted in other figures for clarity. (***a***) The change of torque in fully hydrogenated graphene annulus with R_{i}=1.5*nm* and R_{o}=4.5*nm* with the rotation angle. (***c***) Wrinkle contour of graphane annulus by coloring each atom according to the out-of-plane displacement. (***d***) The evolution of wrinkle amplitude with rotation angle. (***e***) Wrinkle amplitude contours of graphane annulus with R_i=3*nm*, R_o=9*nm* at 1*K* by coloring each atom according to the out-of-plane displacement.

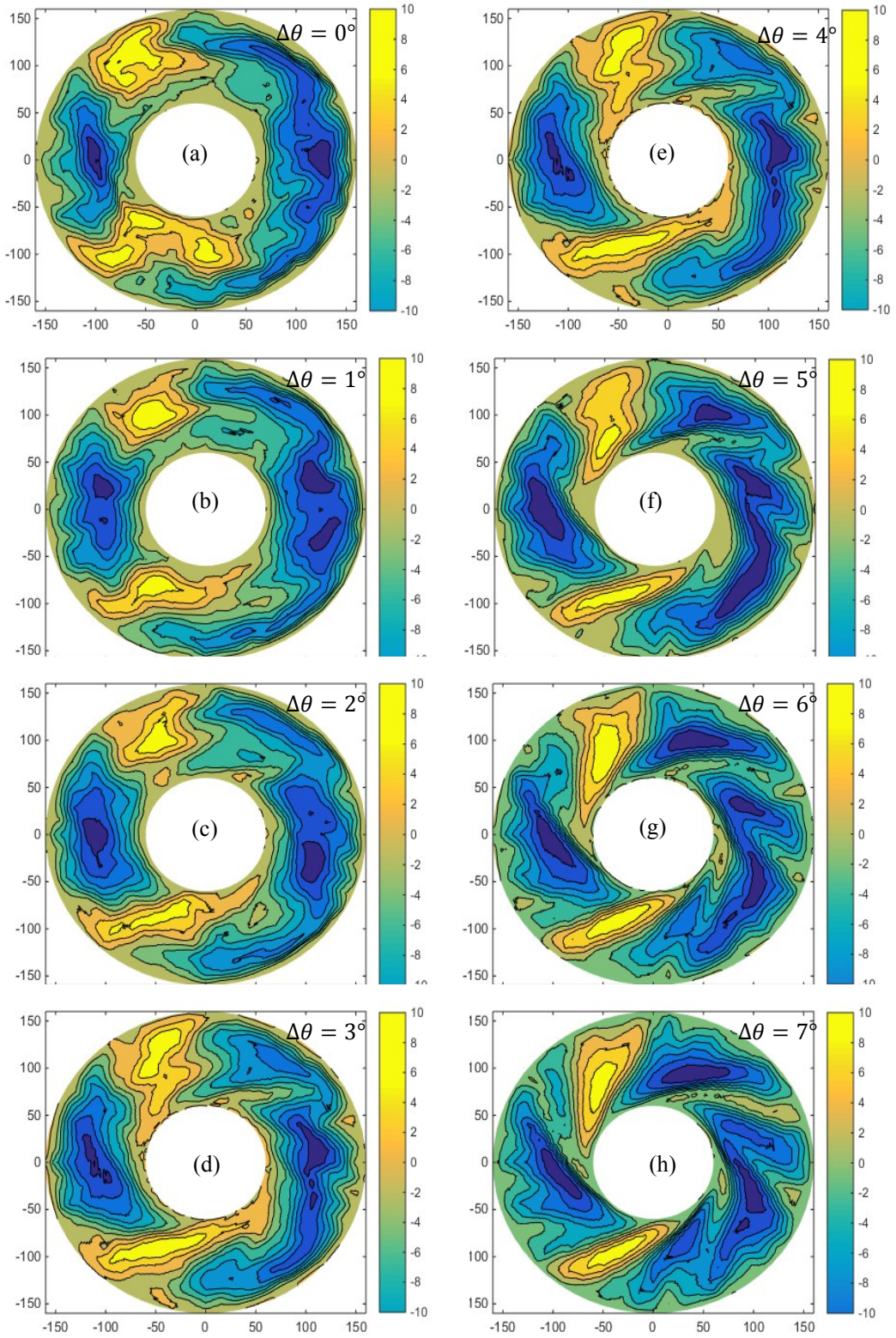

Fig. S2 Out-of-plane deformations of the graphene layer. (a-h) Contour maps of circular hydrogenated graphene annulus under torsion angle $\Delta\theta$ ranging from 0º to 7º. The surface morphology of relaxed

graphene is noticed to be different with that of graphene under in-plane rotation. Hydrogenated graphene at $\Delta\theta$=0° has random out-of-plane deformation pattern while annulus at $\Delta\theta$>3° shows unusual spiral wrinkling patterns.

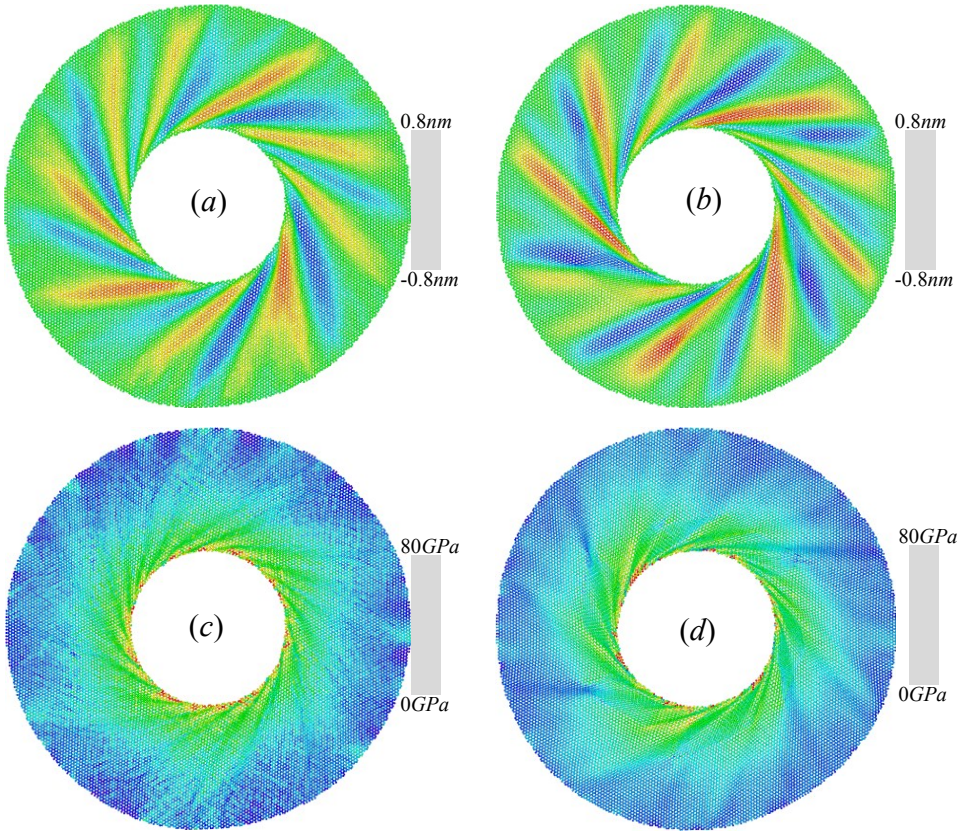

Fig. S3 Enhanced out of plane deformation induced change of in-plane stress distribution. (*a*-*b*) Wrinkle amplitude contours of hydrogenated graphene annulus with hydrogenation ratio *H*=10% and100% at the critical rotation angle, and (*c*-*d*) the corresponding stress distributions for circular shear stress. Graphane annulus with larger wrinkle amplitude shows more severe wrinkling induced local stress state conversion, which agrees with the study reported by Li *et al*[1].

References

1. Y. Li, Q. Lin and D. Cui, *Sci. Rep.*, 2017, 7, 41767.