Supplementary Information

Sign-Tunable Poisson's Ratio in Semi-Fluorinated Graphene

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Figure S1. Electronic band structure of C_2F boat structure (a) without strain, with ZZ strain of (b) 9%, (c) 16% and (d) 24%, and AC strain of (e) 5% and (f) 10%. The red lines denote the Fermi level, which is set to the valence band maximum.



Figure S2. Atomic structure of C_2F boat structure (a) without strain, with ZZ strain of (b) 9%, (c) 16% and (d) 24%, and AC strain of (e) 5% and (f) 10%.



Figure S3. Phonon bands of C_2H boat structure (a) without strain and (b) ZZ strain of 18%, respectively. Imaginary phonon frequencies (conventionally drawn as negative) appear at ZZ strain of 18%.



Figure S4. (a) Stress-strain relationship of C_2H boat structure under uniaxial stress along zigzag direction. (b) Transverse strain (ϵ_{trans}) and Poisson's ratio as a function of the ZZ strain.



Figure S5. (a) Transverse strain (ε_{trans}) as a function of the axial strain (ε_{axial}) for graphene under ZZ and AC stress. (b) Poisson's ratio as a function of the axial strain for graphene under ZZ and AC stress. The vertical red and black dash lines denote the critical AC and ZZ strains of 19.4% and 26.6%, respectively, whose values are from Ref. 56.