Supplementary Information

Investigation of mechanical properties and structural integrity of graphene aerogels via molecular dynamics simulations

Bowen Zheng[1], Chen Liu[2], Zhou Li[3,4], Carlo Carraro[4], Roya Maboudian[4], Debbie G. Senesky[3,5], and Grace X. Gu[1,*]

[1]Department of Mechanical Engineering, University of California, Berkeley, CA 94720, United States
[2]Department of Mechanical Engineering, Stanford University, CA 94305, United States
[3]Department of Aeronautics & Astronautics, Stanford University, CA 94305, United States
[4]Department of Chemical and Biomolecular Engineering, and Berkeley Sensor & Actuator Center, University of California, Berkeley, CA 94720, United States
[5]Department of Electrical Engineering, Stanford University, CA 94305, United States

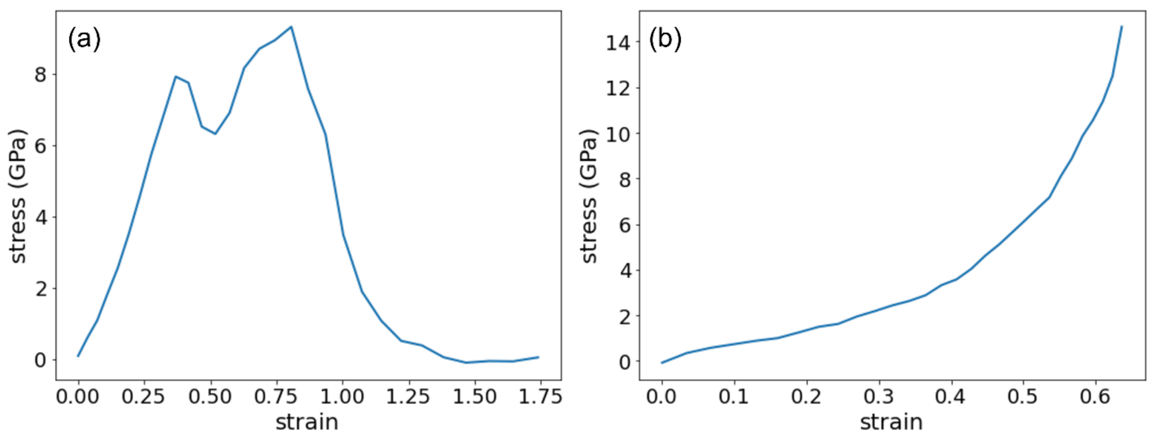

Figure S1. Stress-strain curves where $N_{\text{flake}} = 200$, $N_{\text{inc}} = 200$, $\sigma = 5.0$ Å, $N_{\text{cycles}} = 10$, and $T_{\text{A}} = 2000$ K. Stress-strain curves under (a) tension and (b) compression.

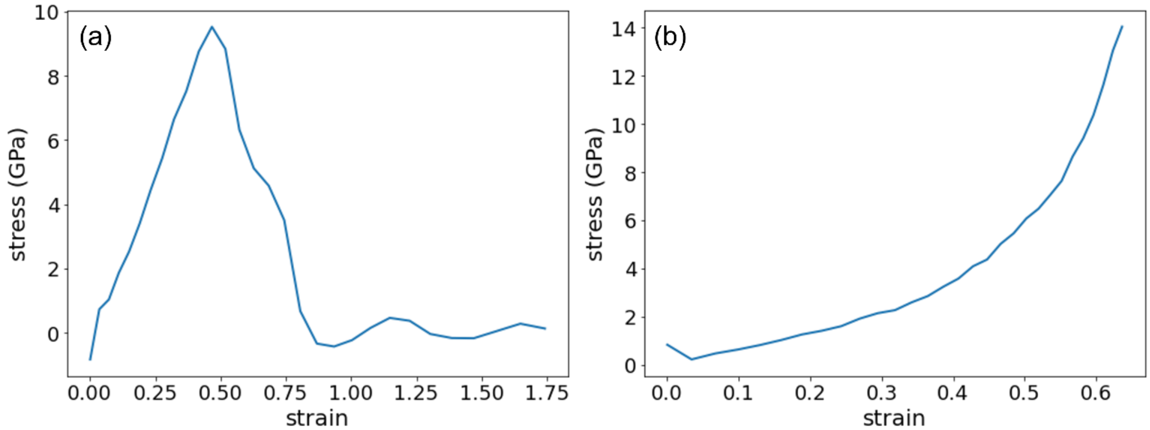

Figure S2. Stress-strain curves without the relaxation process after annealing cycles where $N_{\text{flake}} = 200$, $N_{\text{inc}} = 200$, $\sigma = 5.0$ Å, $N_{\text{cycles}} = 10$, and $T_{\text{A}} = 2000$ K. Stress-strain curves under (a) tension and (b) compression.

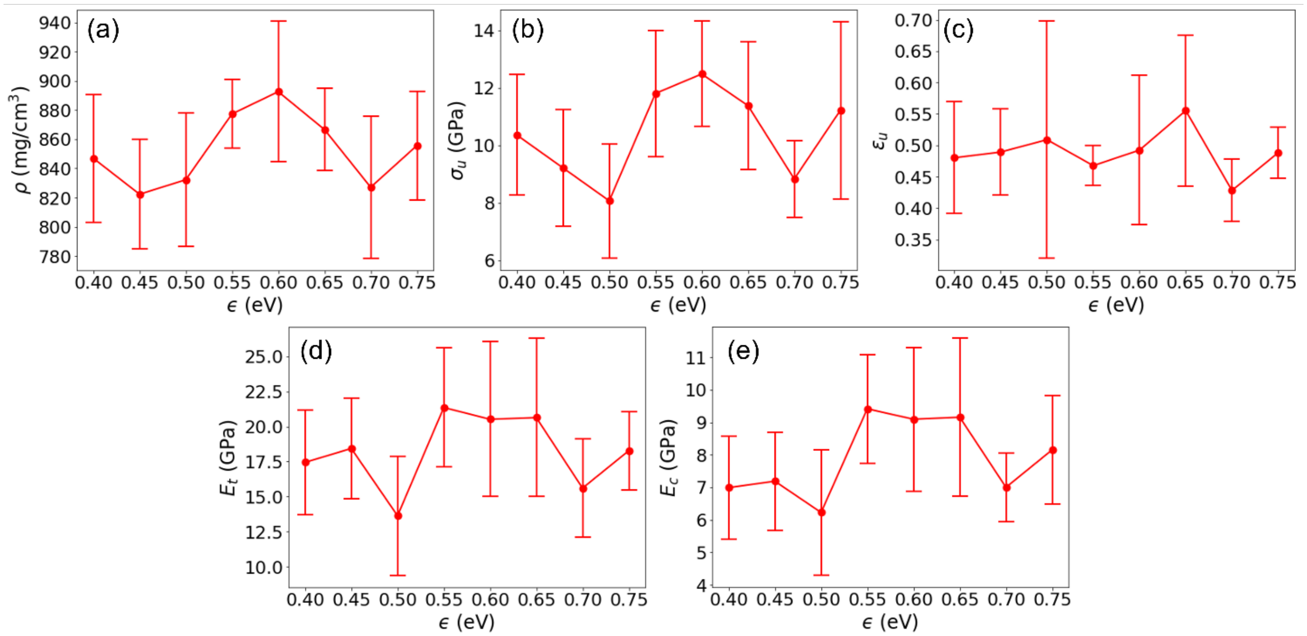

Figure S3. Mechanical properties of GA as a function of ϵ. (a) Density ρ, (b) tensile strength σ_{u}, (c) tensile failure strain ε_{u}, (d) tensile and (e) compressive moduli E_{t} and E_{c} of GA as a function of ϵ.

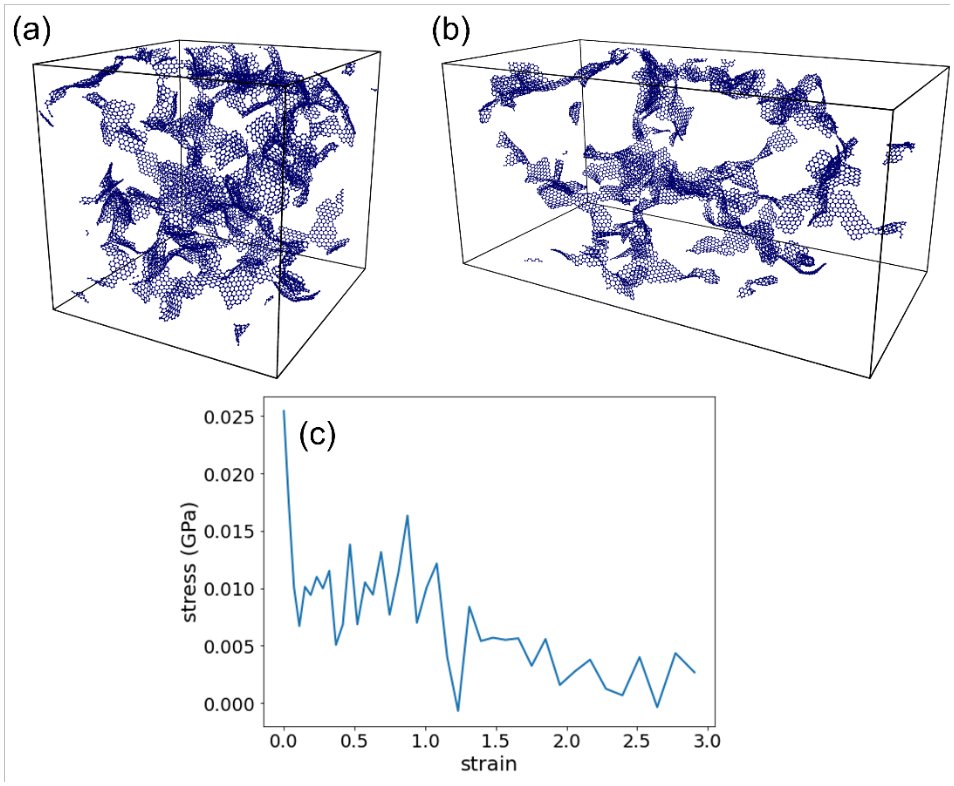

Figure S4. Disconnected GA structure. The structure when (a) unloaded and (b) under tension. (c) Stress-strain relation of the GA under tension.

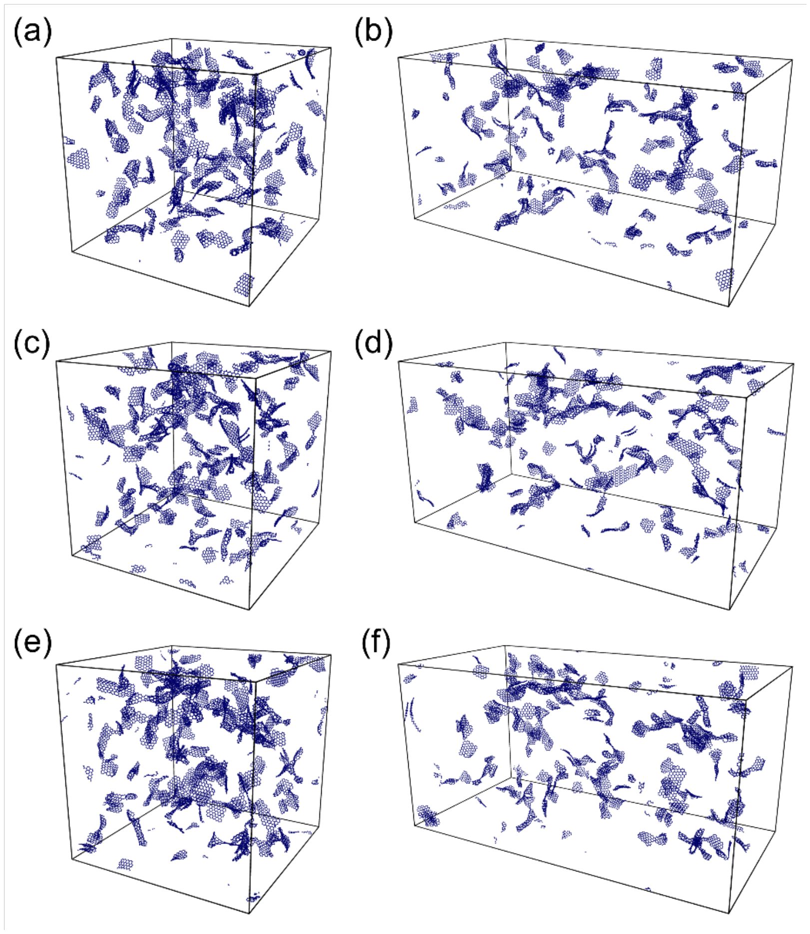

Figure S5. GA structure where $N_{\text{flake}} = 200$, $R = 5.0$, $\sigma = 15.0$ Å, and $T_{\text{A}} = 2000$ K under various numbers of annealing cycles. Initial structure and the structure under tension of GAs prepared with (a) 10, (b) 20, and (c) 50 annealing cycles. $N_{\text{bond/atom}}$ for (a-c) are 1.384, 1.386, 1.389, respectively.

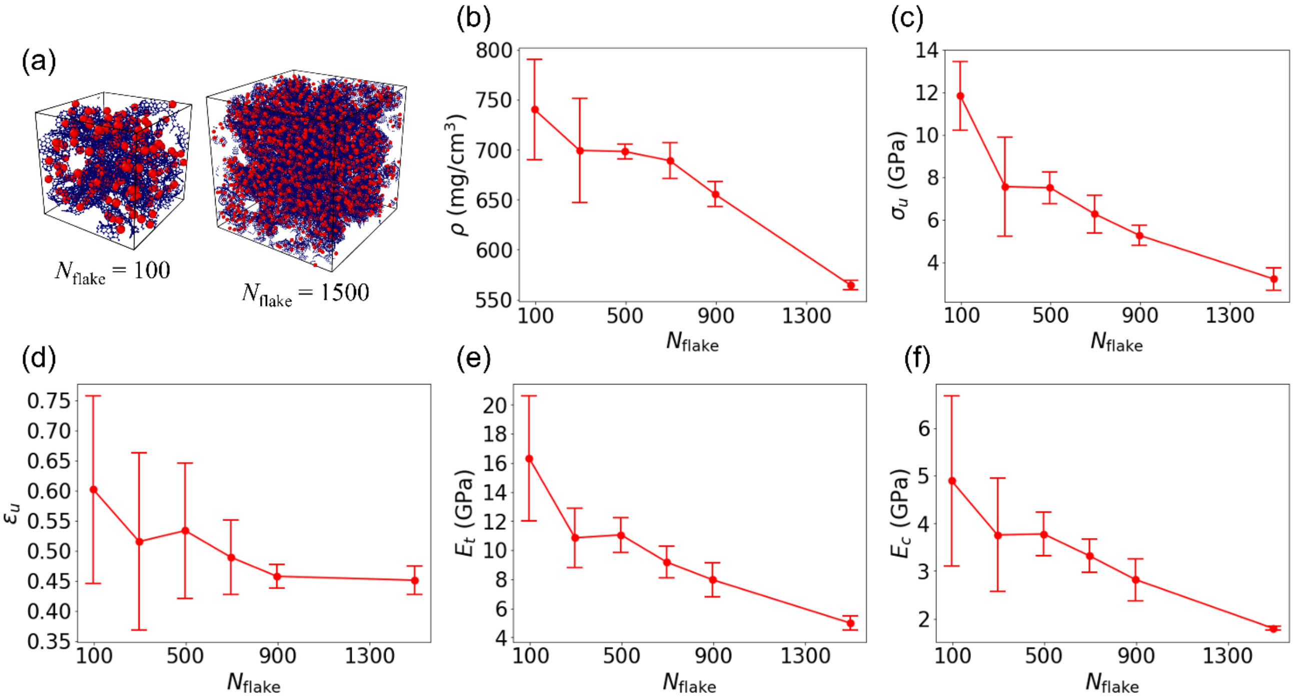

Figure S6. Mechanical properties of GA as a function of N_{flake}. (a) Illustration of the effect of N_{flake}. (b) Density ρ, (c) tensile strength σ_{u}, (d) tensile failure strain ε_{u}, (e) tensile and (f) compressive moduli E_{t} and E_{c} of GA as a function of N_{flake}.

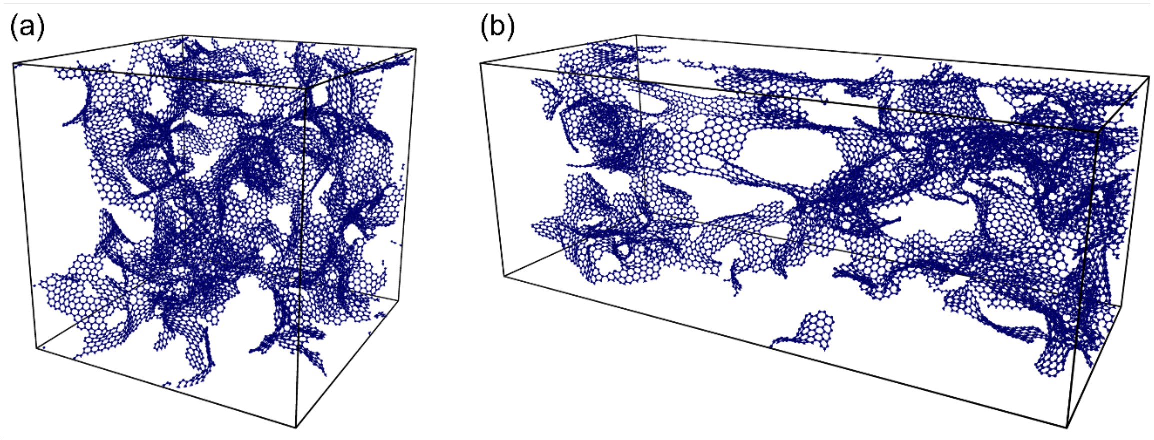

Figure S7. GA structure where $N_{\mathrm{flake}} = 200$, $R = 1.0$, $\sigma = 13.0$ Å, and $T_{\mathrm{A}} = 2000$ K. The structure when (a) unloaded and (b) subject to tension.

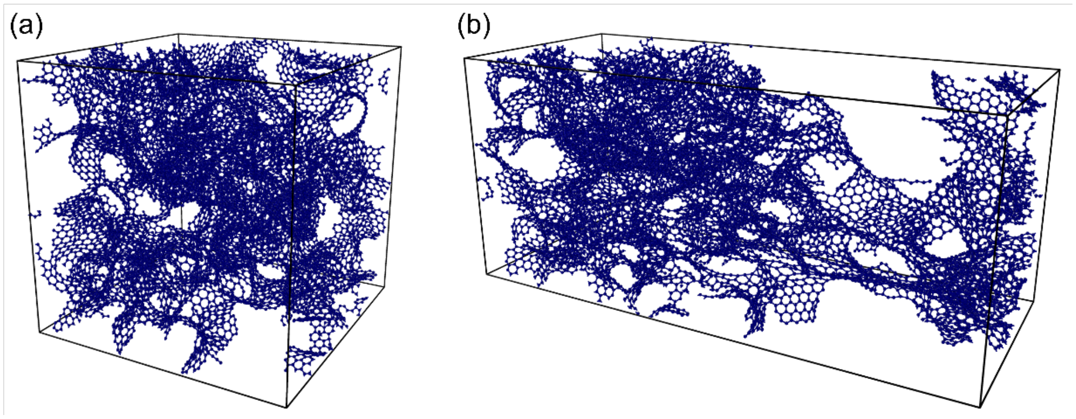

Figure S8. GA structure where $N_{\text{flake}} = 200$, $R = 5.5$, $\sigma = 5.0$ Å, and $T_{\text{A}} = 2000$ K. The structure when (a) unloaded and (b) subject to tension.

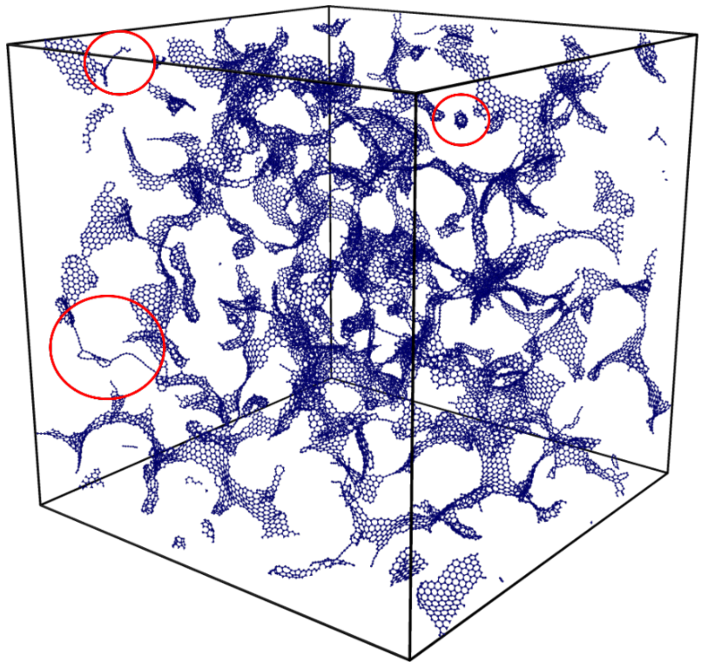

Figure S9. GA structure formed with annealing temperature $T_{\mathrm{A}} = 4000$ K where bond breakings and thermally unstable behavior are observed. Problematic geometries are circled.

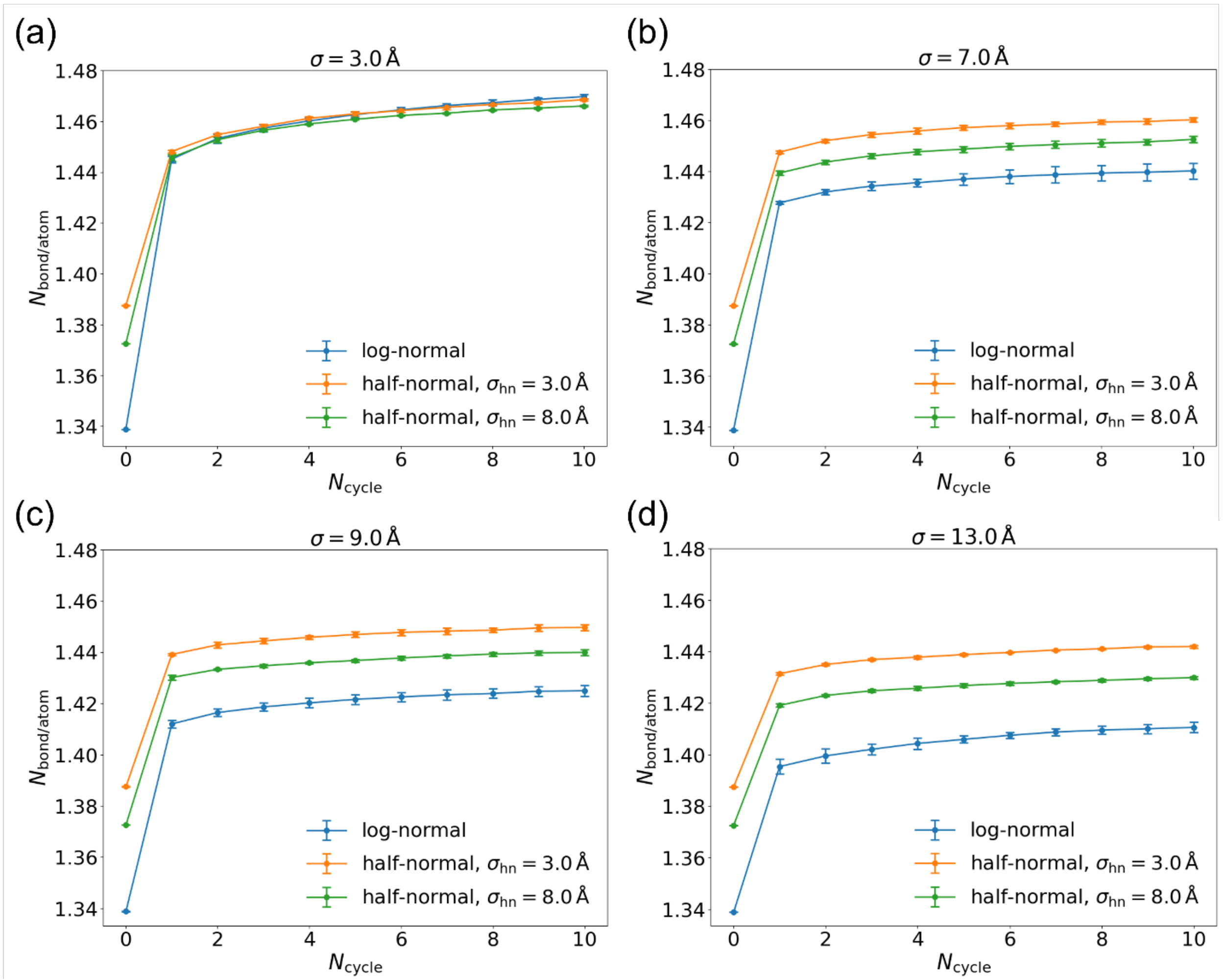

Figure S10. GA connectivity property under different distributions of graphene flake side length L. $N_{\mathrm{bond/atom}}$ versus N_{cycle} plots with (a) $\sigma = 3.0$ Å, (b) $\sigma = 7.0$ Å, (c) $\sigma = 9.0$ Å, and (d) $\sigma = 13.0$ Å

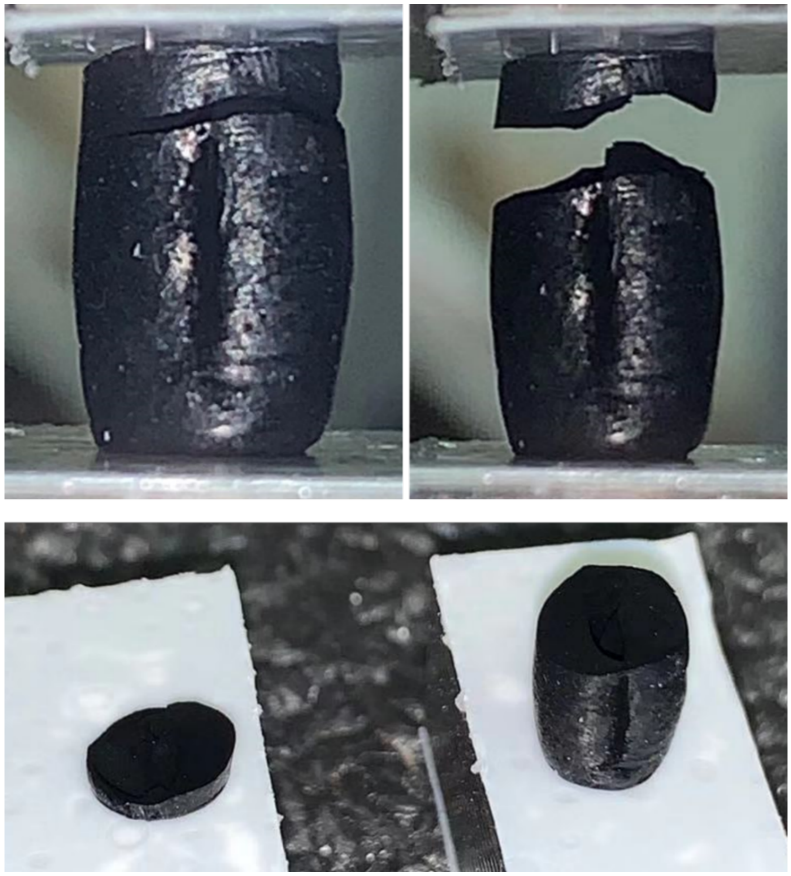

Figure S11. Images of GA showing catastrophic failure during tensile test. Compression tests were performed on dynamic mechanical analysis (DMA, TA Instrument Q800). A preload of 10 mN was applied on the GA samples to assure full contact. The samples were compressed to 80 % strain with a loading rate of 10 % strain/min. Tension tests were performed on universal testing machines (Instron) with a loading rate of 10 % strain/min.

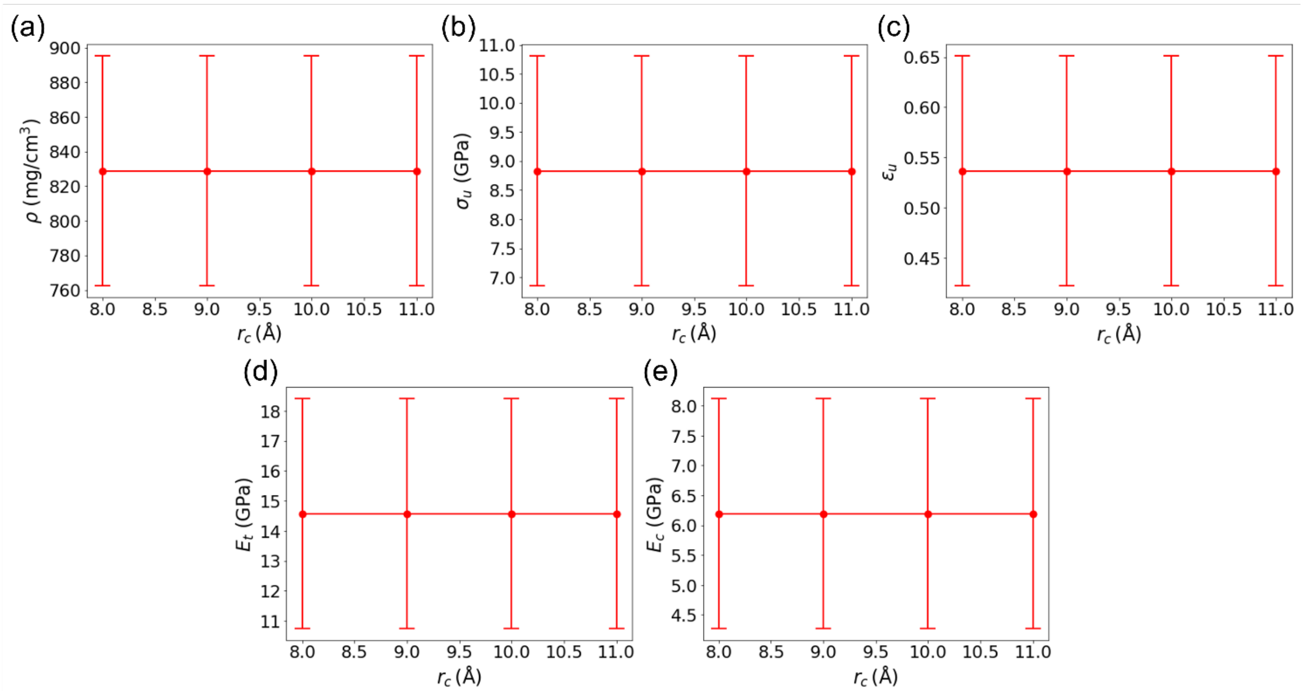

Figure S12. Mechanical properties of GA as a function of the cutoff distance r_c. (a) Density ρ, (b) tensile strength σ_u, (c) tensile failure strain ε_u, (d) tensile and (e) compressive moduli E_t and E_c of GA as a function of r_c. LAMMPS performances for $r_c = 8.0, 9.0, 10.0$ and 11.0 Å are 15.288, 14.791, 13.595 and 12.416 ns/day, respectively.