

Supplementary Information for

Negative Poisson's ratio and high-mobility transport anisotropy
in SiC₆ siligraphene

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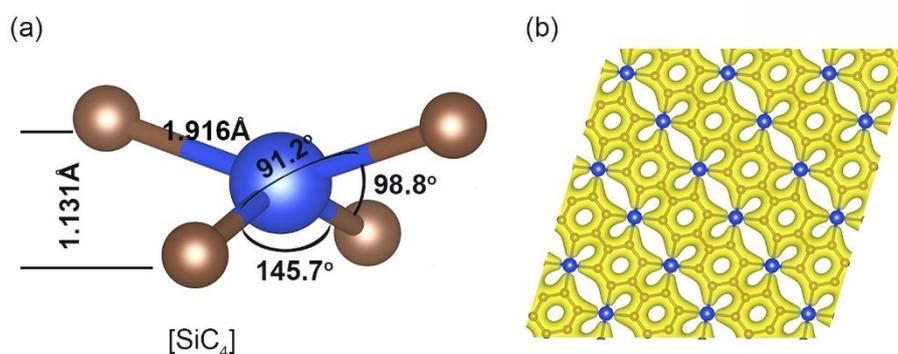


Figure S1 (a) the structure parameter of the [SiC₄] unit in the SiC₆ siligraphene and (b) the isosurfaces of the total electron density of SiC₆ siligraphene with the isovalue of 0.08 e/Å³. The large blue balls represent silicon atoms.

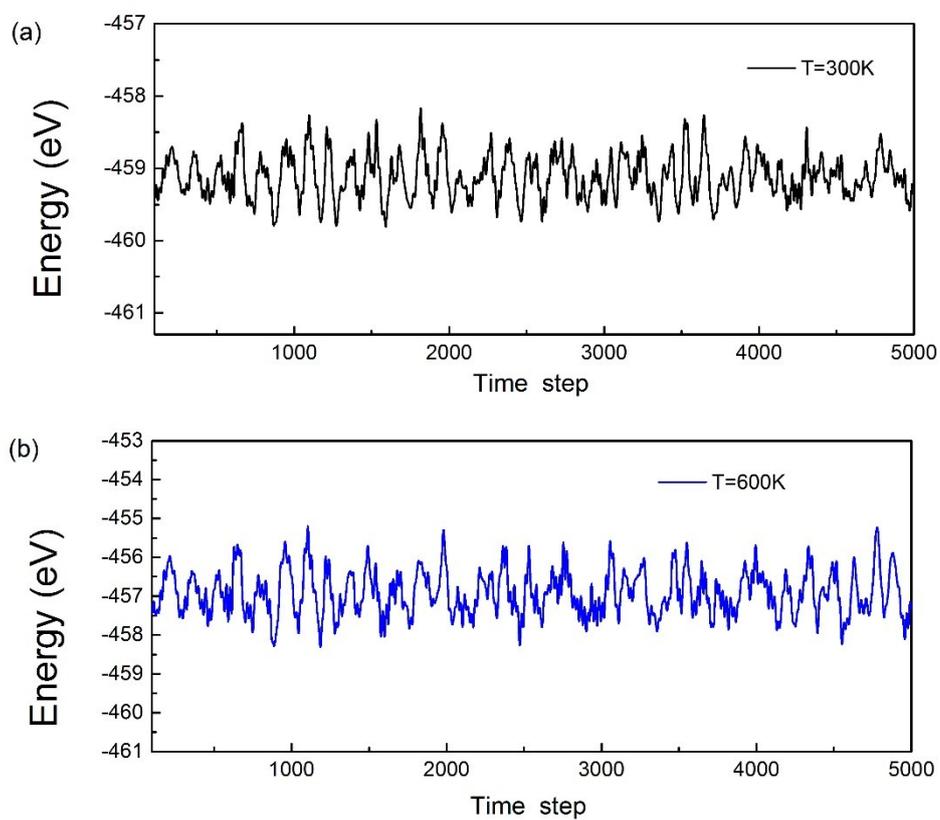


Figure S2 The time evolution of total energy of the SiC₆ siligraphene at the temperatures of (a) 300K and (b) 600 K, obtained by ab initio molecular dynamics simulations. The simulation lasted for 5000 steps with a time step of 0.5 fs.

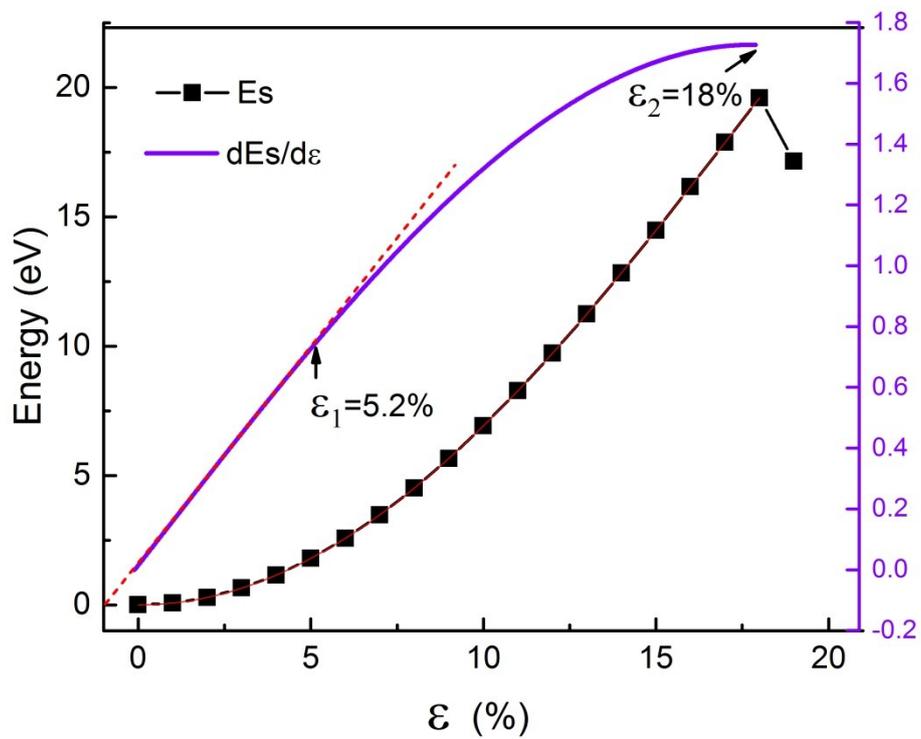


Figure S3 The strain energy and its derivative of the SiC₆ siligraphene under uniform expansion. The critical strain between elastic and plastic regions is about 18%.