Supplementary material:

Microscopic origin of graphene nanosheets derived from coal-tar pitch by

treating Al_4C_3 as the intermediate

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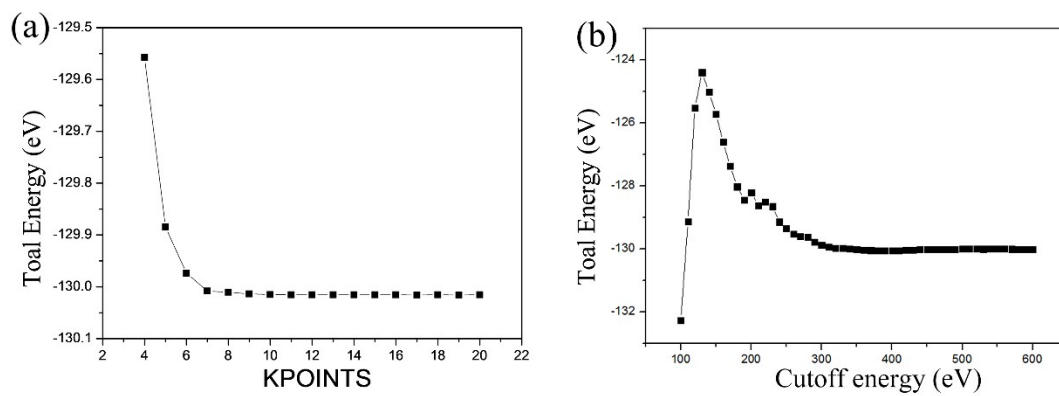Corresponding authors: bssa@fzu.edu.cn (B. Sa); linqilang@fzu.edu.cn (Q. Lin).

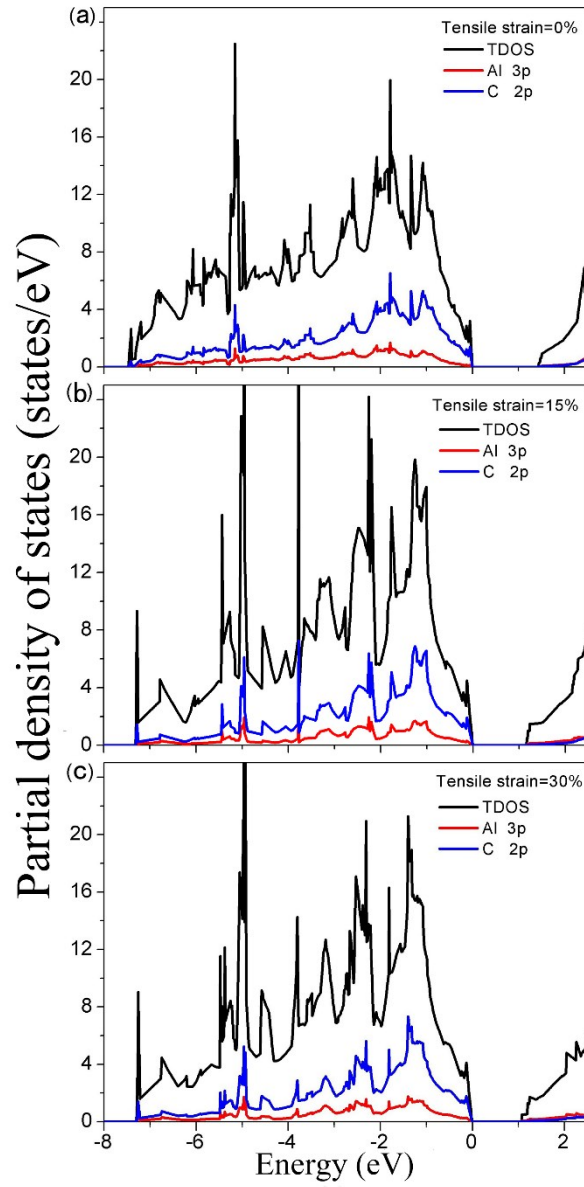Figure S1. (a) The KPOINTS mesh and (b) cutoff energy convergence test results

Figure S2. The calculated total and partial density of states of Al_4C_3 under (a) 0%, (b) 15% and (c) 30% tensile strain along [0001] direction by DFT-D3 approach.
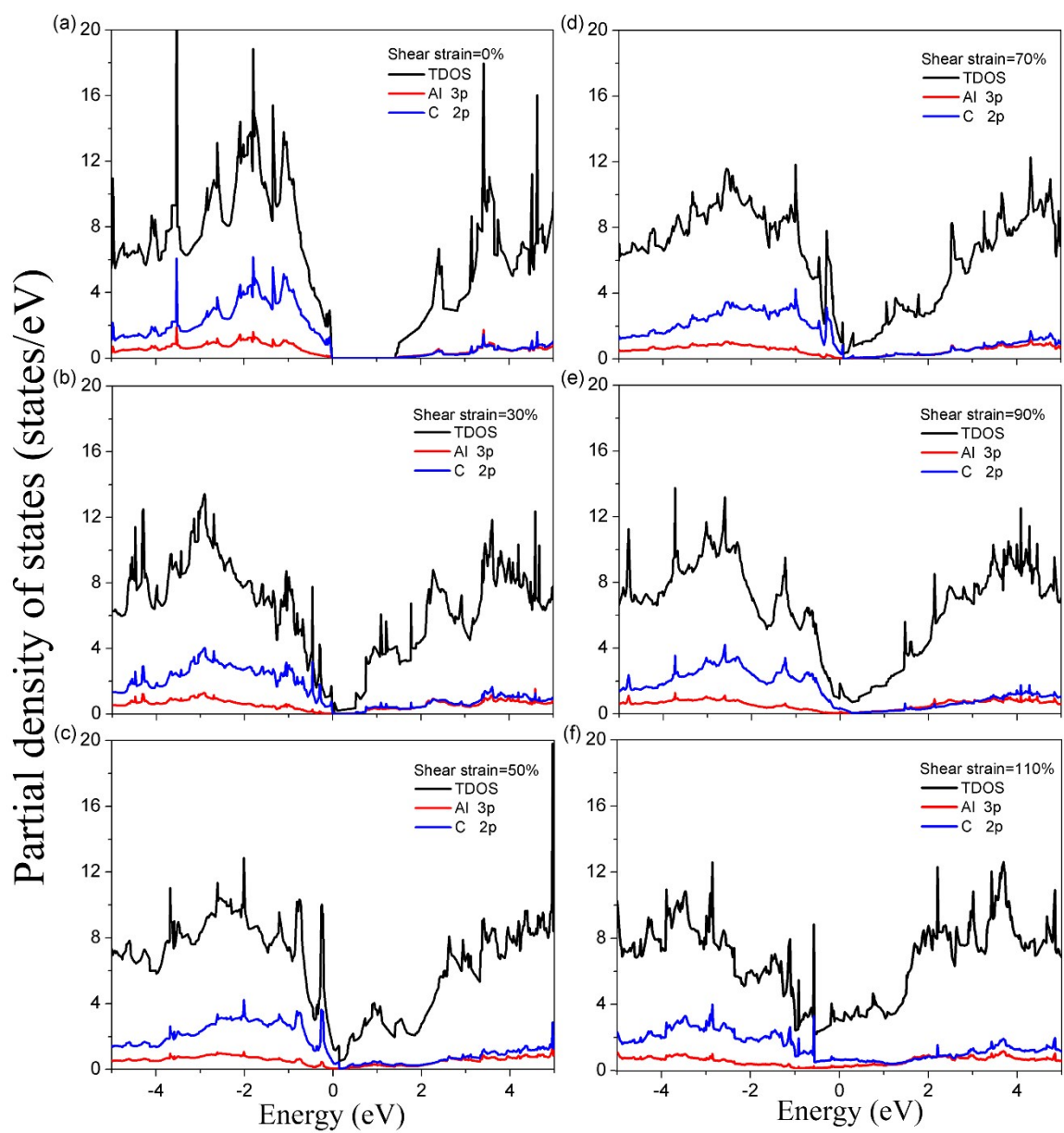
Figure S3. The calculated total and partial density of states of Al_4C_3 under (a) 0%, (b) 30%, (c) 50%, (d) 70%, (e) 90% and (f) 110% shear strain along the (0001)[110] direction using DFT-D3 functional.