

Supporting Information

Mechanical engineering effect in electronic and optical properties of graphene nanomeshes

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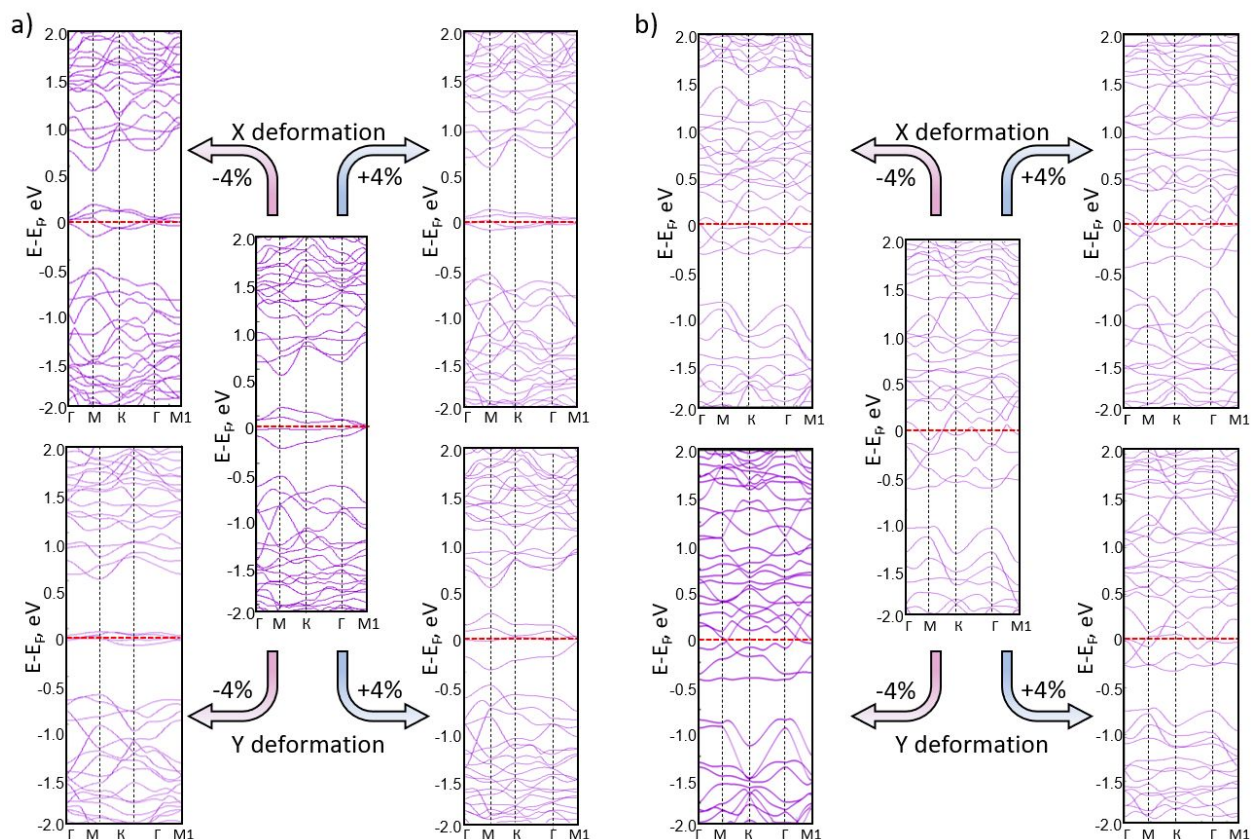


Fig. S1 Band structure evolution of BGS with AB (a) and Moire (b) type of stackings. By red horizontal line, the Fermi energy depicted.

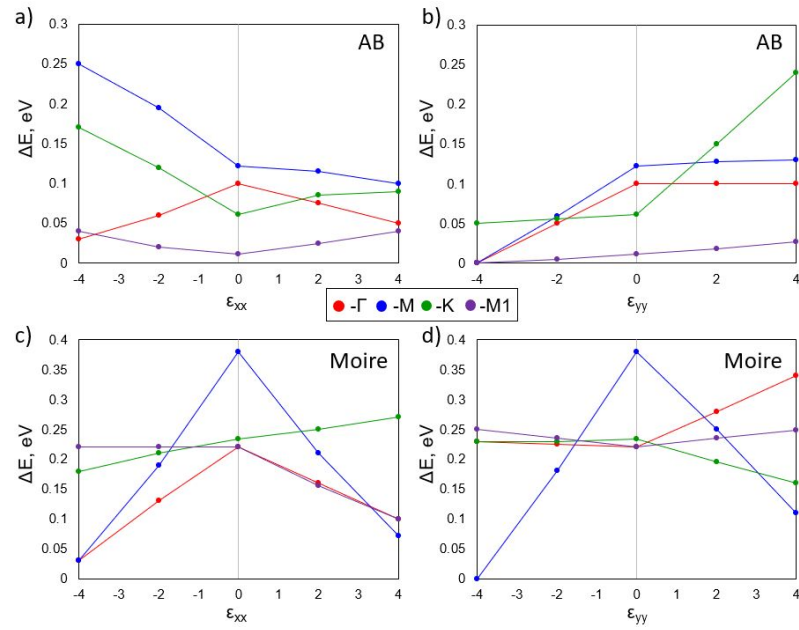


Fig. S2 Dependences of the energy difference between the states in valence and conduction bands in BGNM with AB (a,b) and Moire (c,d) type of stacking deformed along X (a,c) and Y (b,d) directions.

Mechanical properties

Mechanical characteristics of BGNM was calculated using LCAO approach by means of SIESTA software.¹ Calculation of the main elastic moduli of BGNMs were carried out *via* defining the stress-strain curve. The values of elastic moduli were determined as: $C_{11} = \frac{\sigma_1}{\eta_1}$; $C_{12} = \frac{\sigma_1}{\eta_2}$, where σ_i

and η_i are mechanical stress and strain in exact direction. Poisson ration was estimated as ratio between transverse and axial strain during the deformation along X axis.

The 2D linear constants C_{11} and C_{12} have been defined to be 550 GPa and 102 GPa, which are in average the same for all considered BGNMs. Poisson ratio was estimate as about 0.342.

References:

- (1) Soler, J. M.; Artacho, E.; Gale, J. D.; García, A.; Junquera, J.; Ordejón, P.; Sánchez-Portal, D. The SIESTA Method for Ab Initio Order-N Materials Simulation. *Journal of Physics: Condensed Matter* **2002**, *14* (11), 2745–2779. <https://doi.org/10.1088/0953-8984/14/11/302>.