



Supporting Information

for

Strain-induced bandgap engineering in 2D ψ -graphene materials: a first-principles study

Kamal Kumar, Nora H. de Leeuw, Jost Adam and Abhishek Kumar Mishra

Beilstein J. Nanotechnol. **2024**, *15*, 1440–1452. [doi:10.3762/bjnano.15.116](https://doi.org/10.3762/bjnano.15.116)

Additional figures

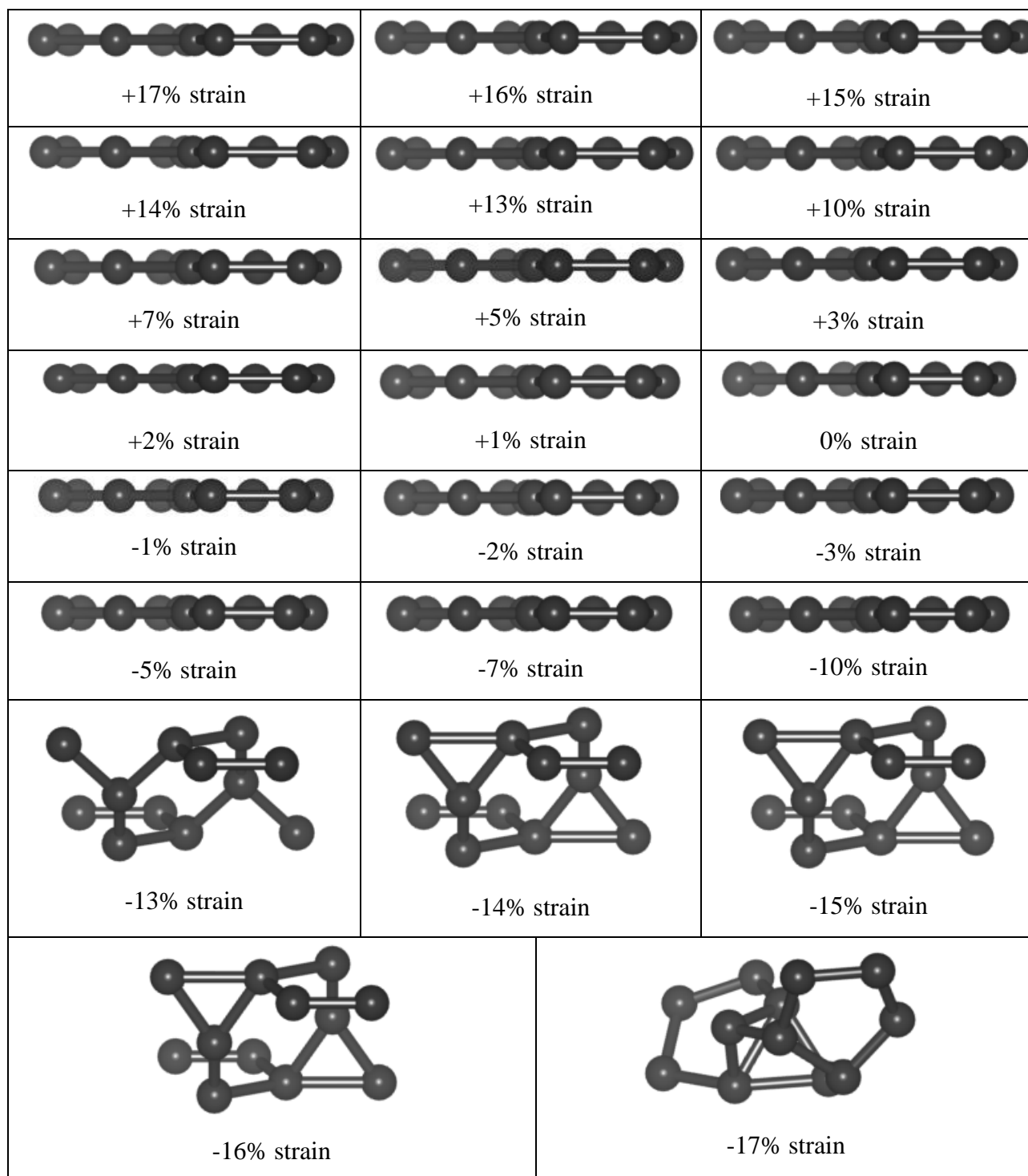


Figure S1: Side view of the relaxed unit cell of ψ -graphene at different strain values.

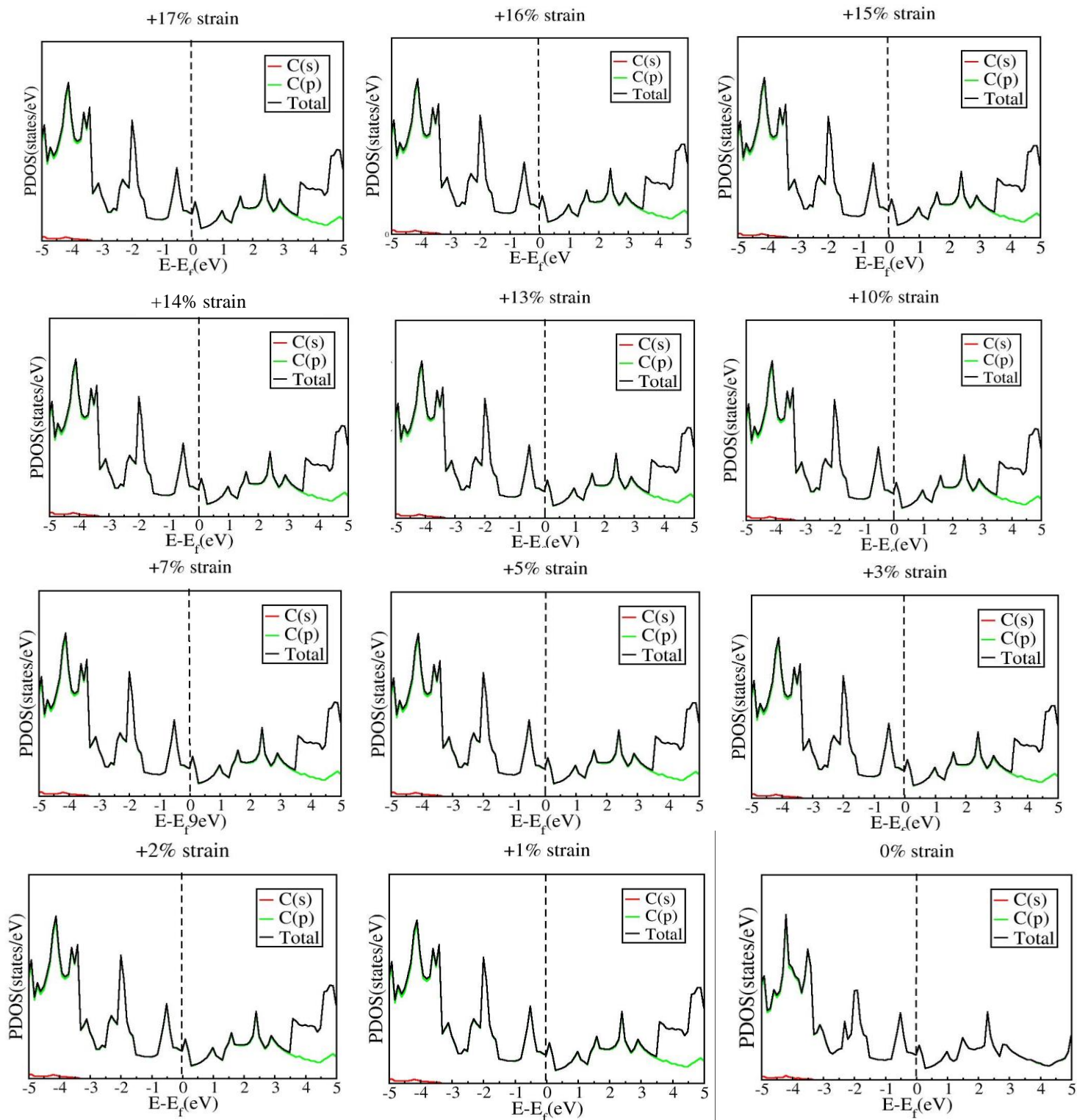


Figure S2: PDOS of ψ -graphene at different values of positive strain.

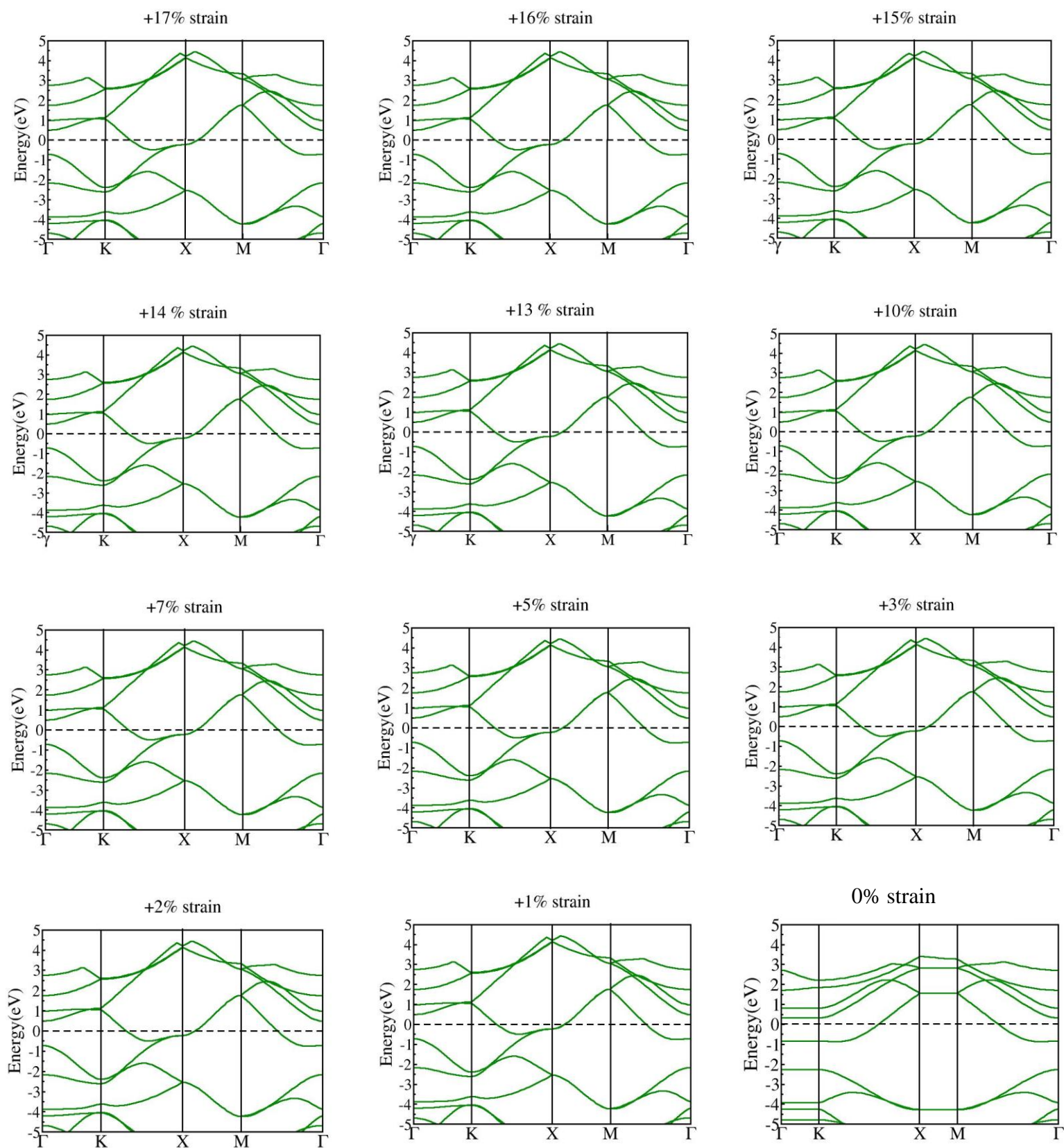


Figure S3: Electronic band structure of ψ -graphene at different values of positive strain.

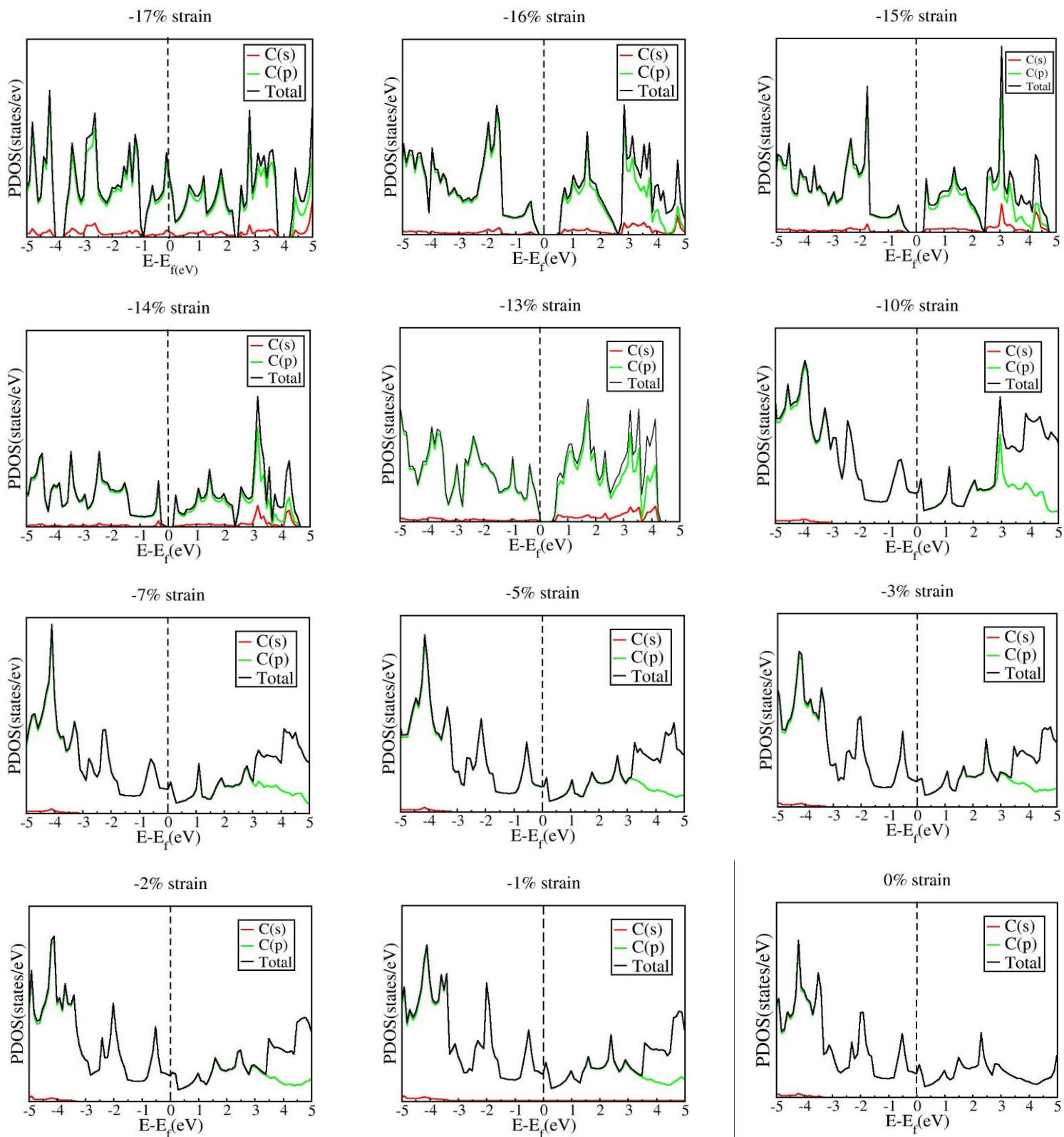


Figure S4: PDOS of ψ -graphene at different values of negative strain.

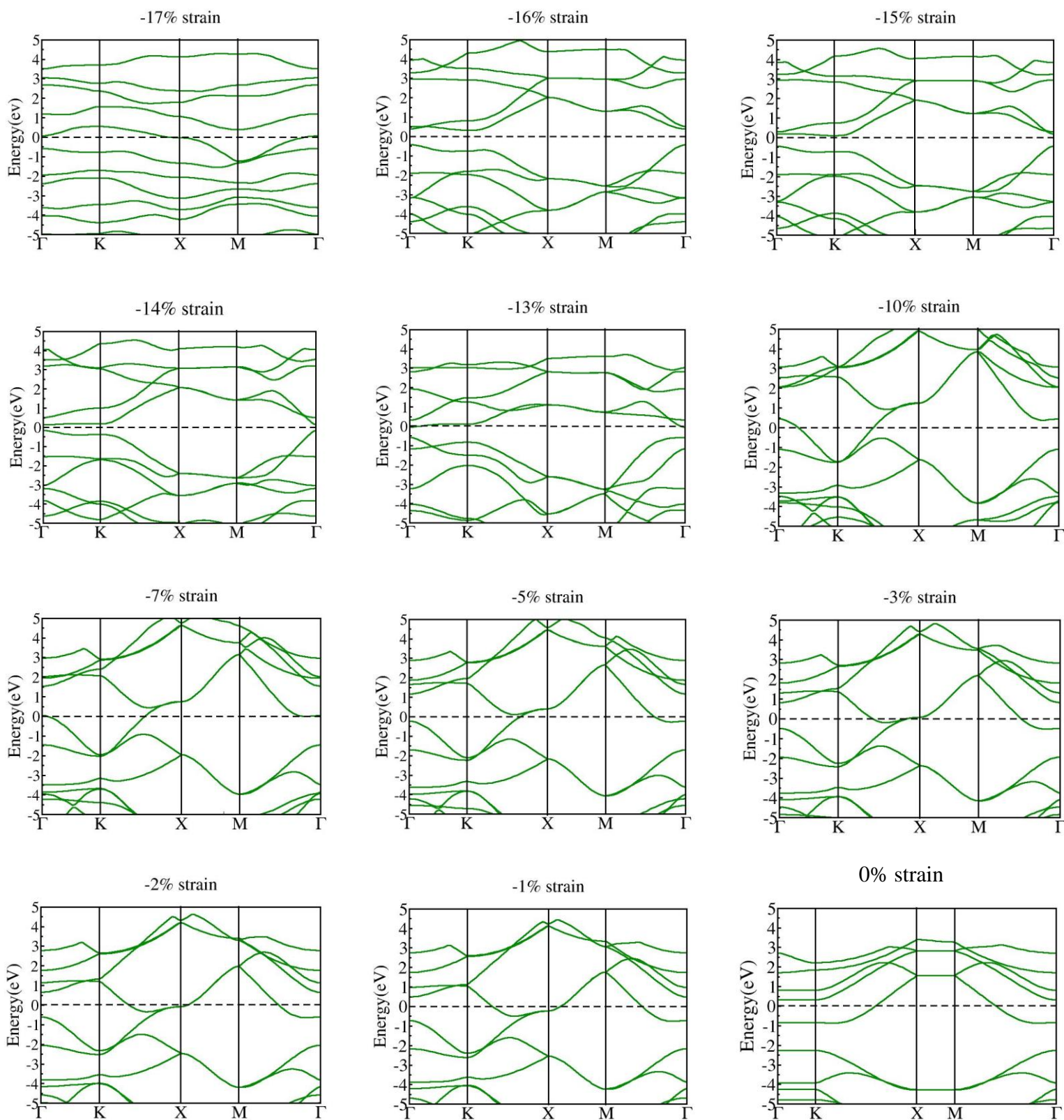


Figure S5: Electronic band structure of ψ -graphene at different values of negative strain.

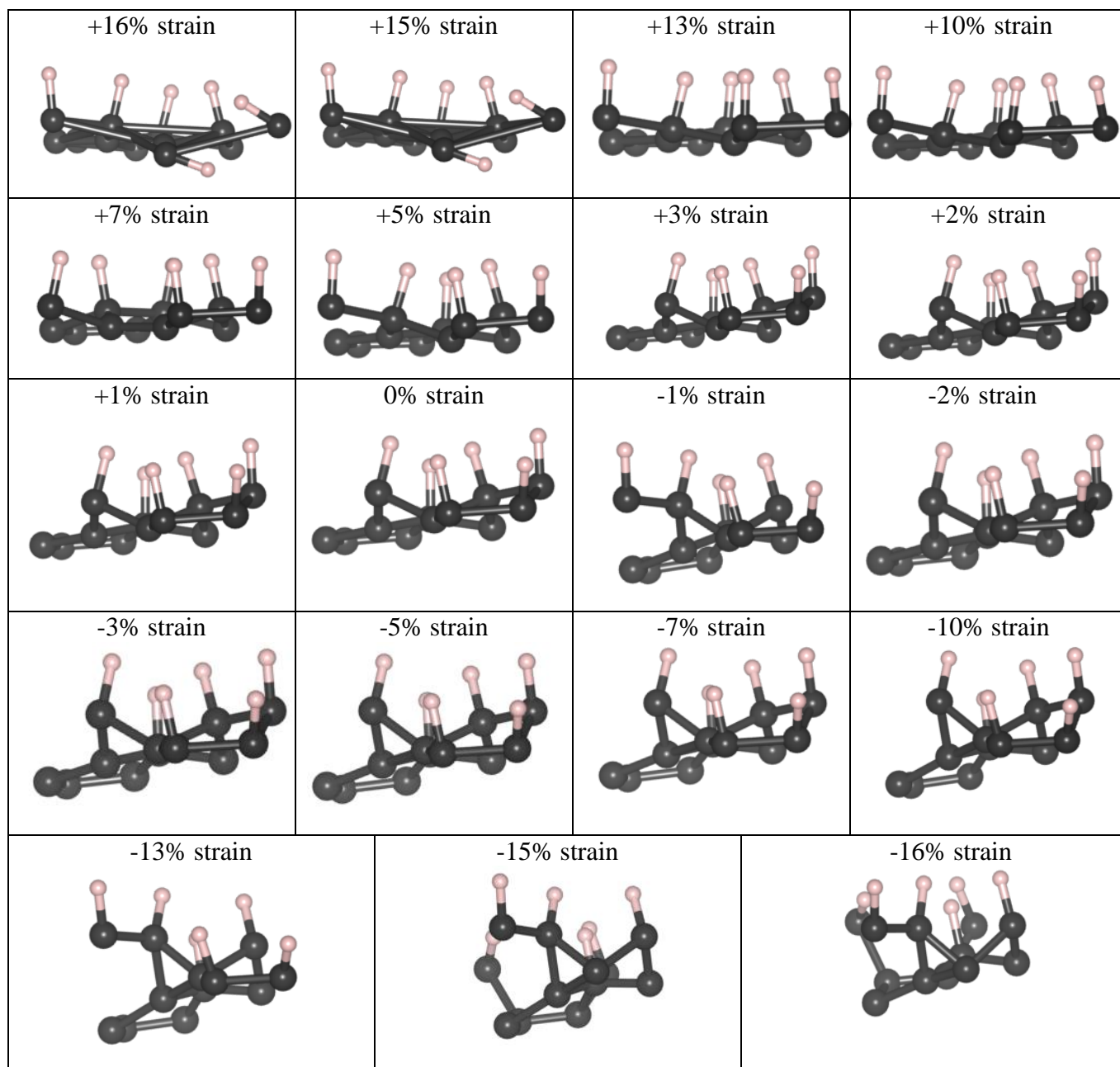


Figure S6: Side view of the relaxed unit cell of ψ -graphene at different strain values.

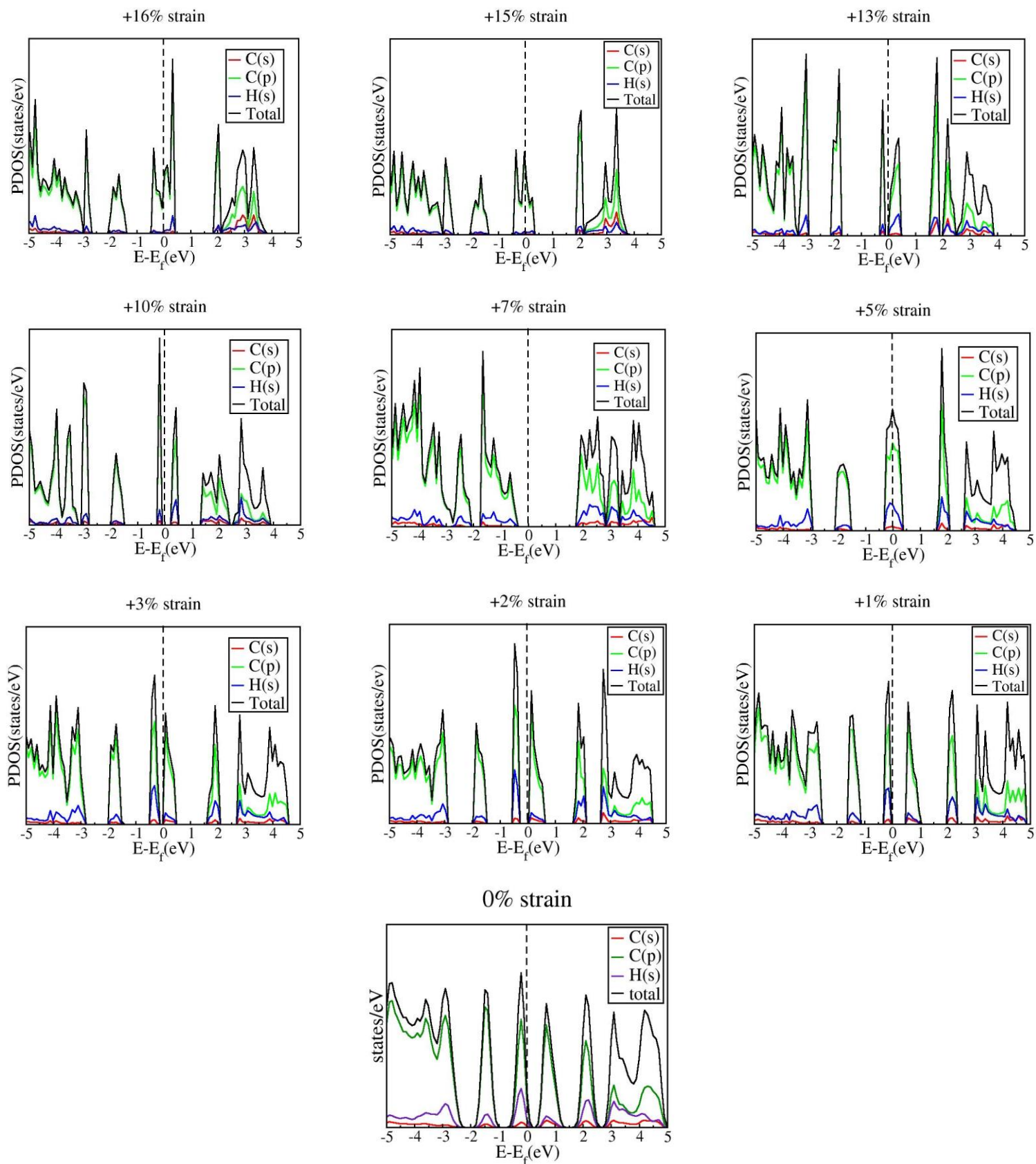


Figure S7: PDOS of ψ -graphene at different values of positive strain.

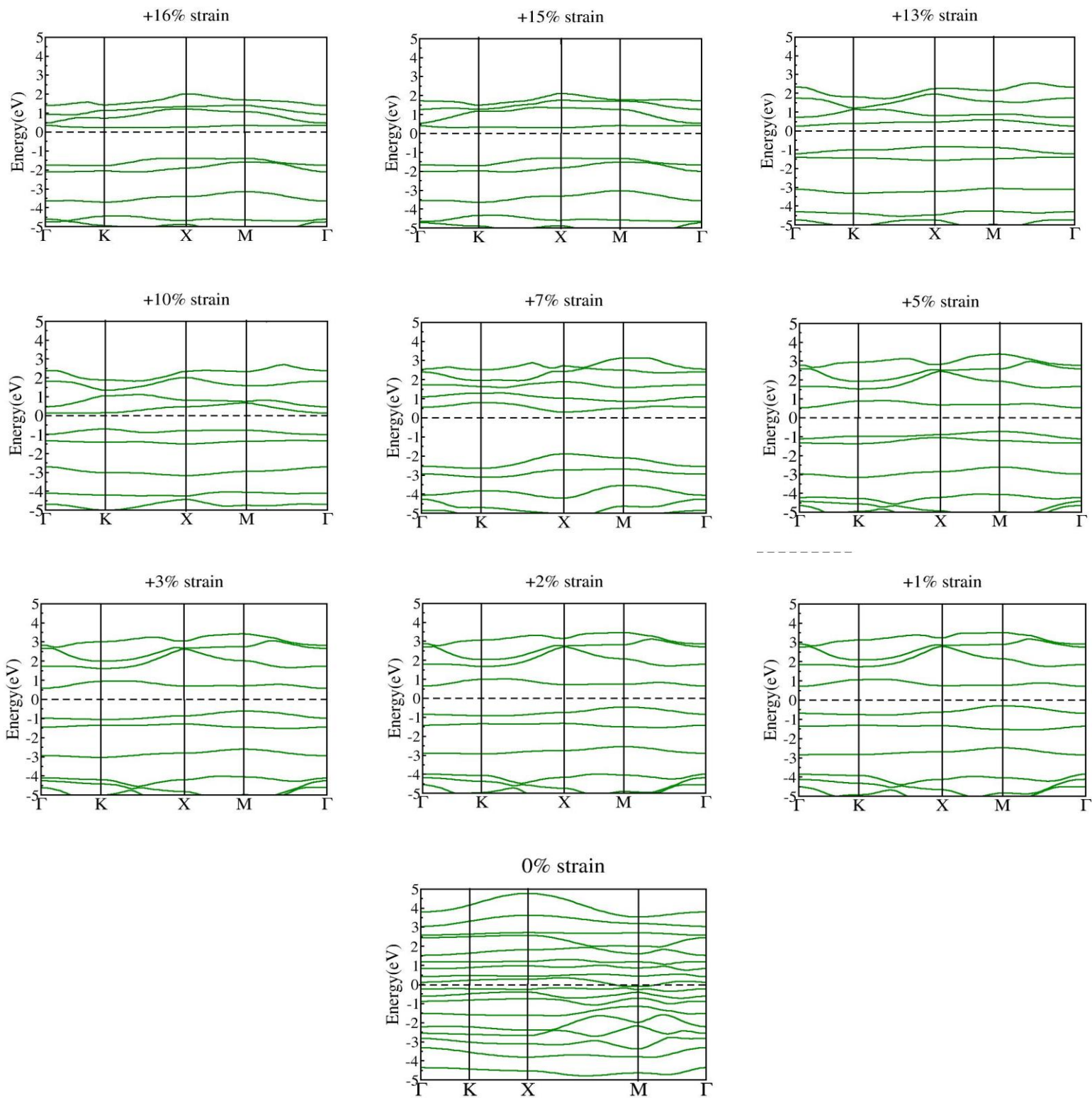


Figure S8: Electronic band structure of ψ -graphene at different values of positive strain.

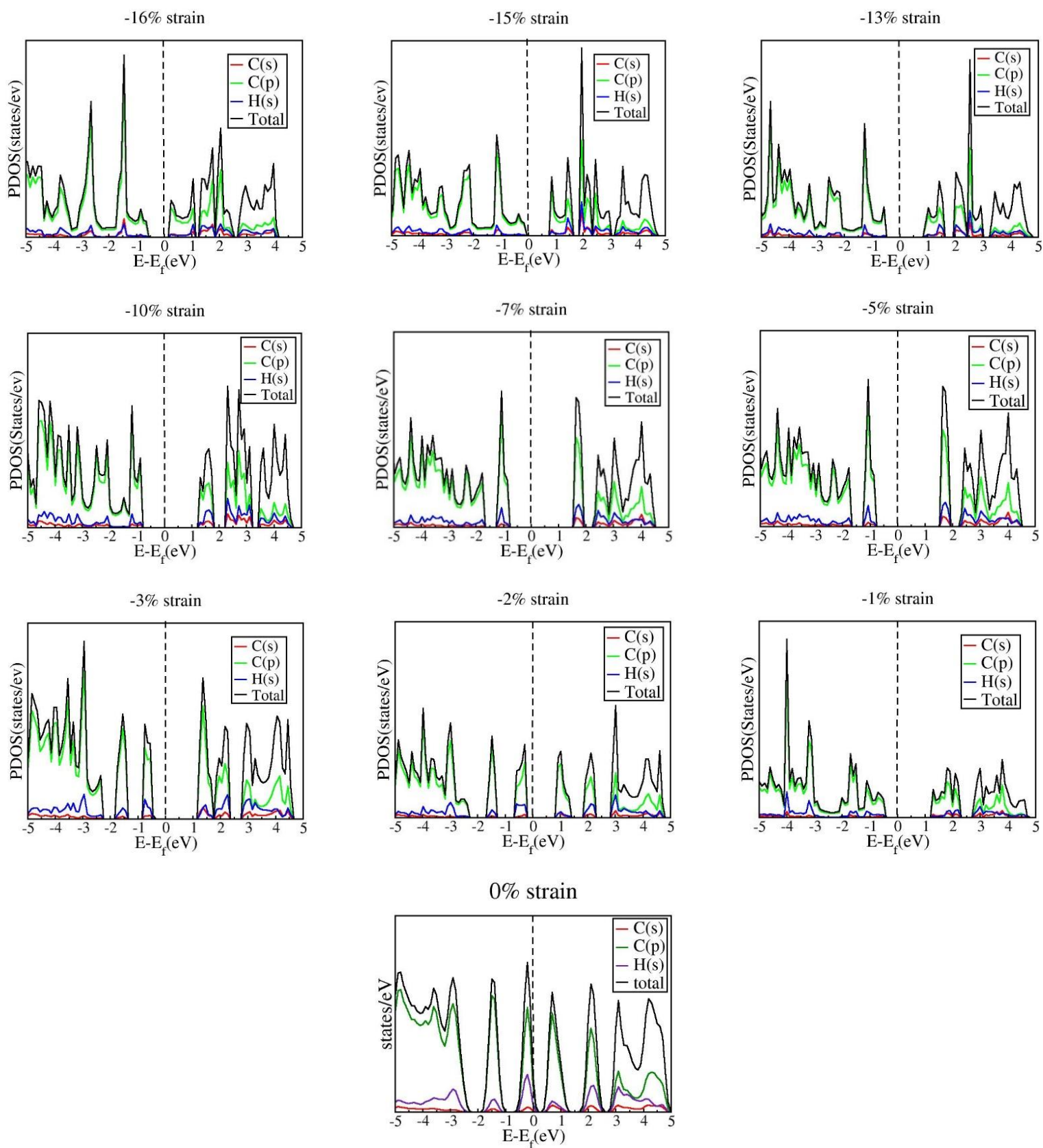


Figure S9: PDOS of ψ -graphene at different values of negative strain.

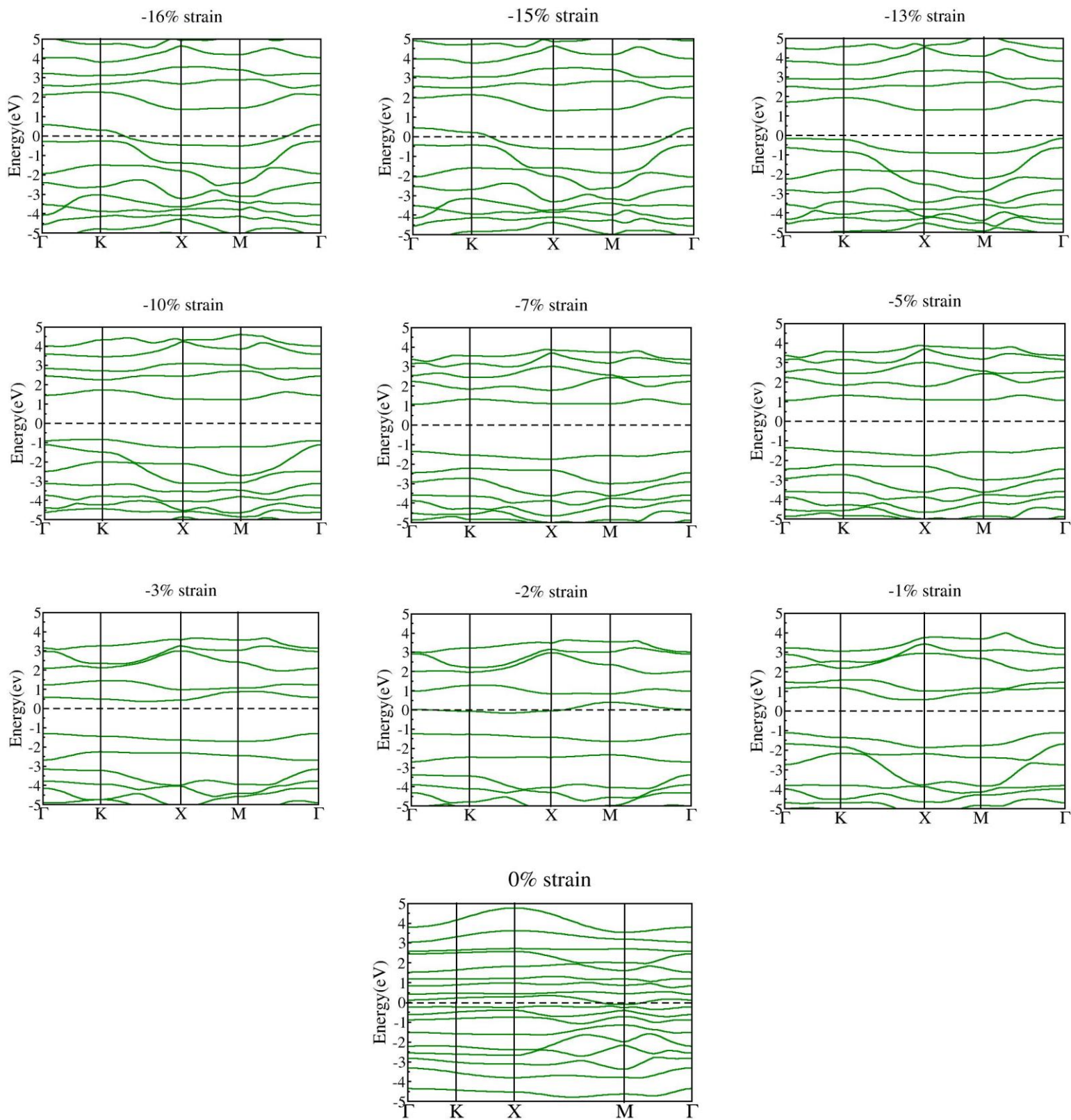


Figure S10: Electronic band structure of ψ -graphene at different values of negative strain.



Figure 11: Side view of the relaxed unit cell of ψ -graphane at different strain levels.

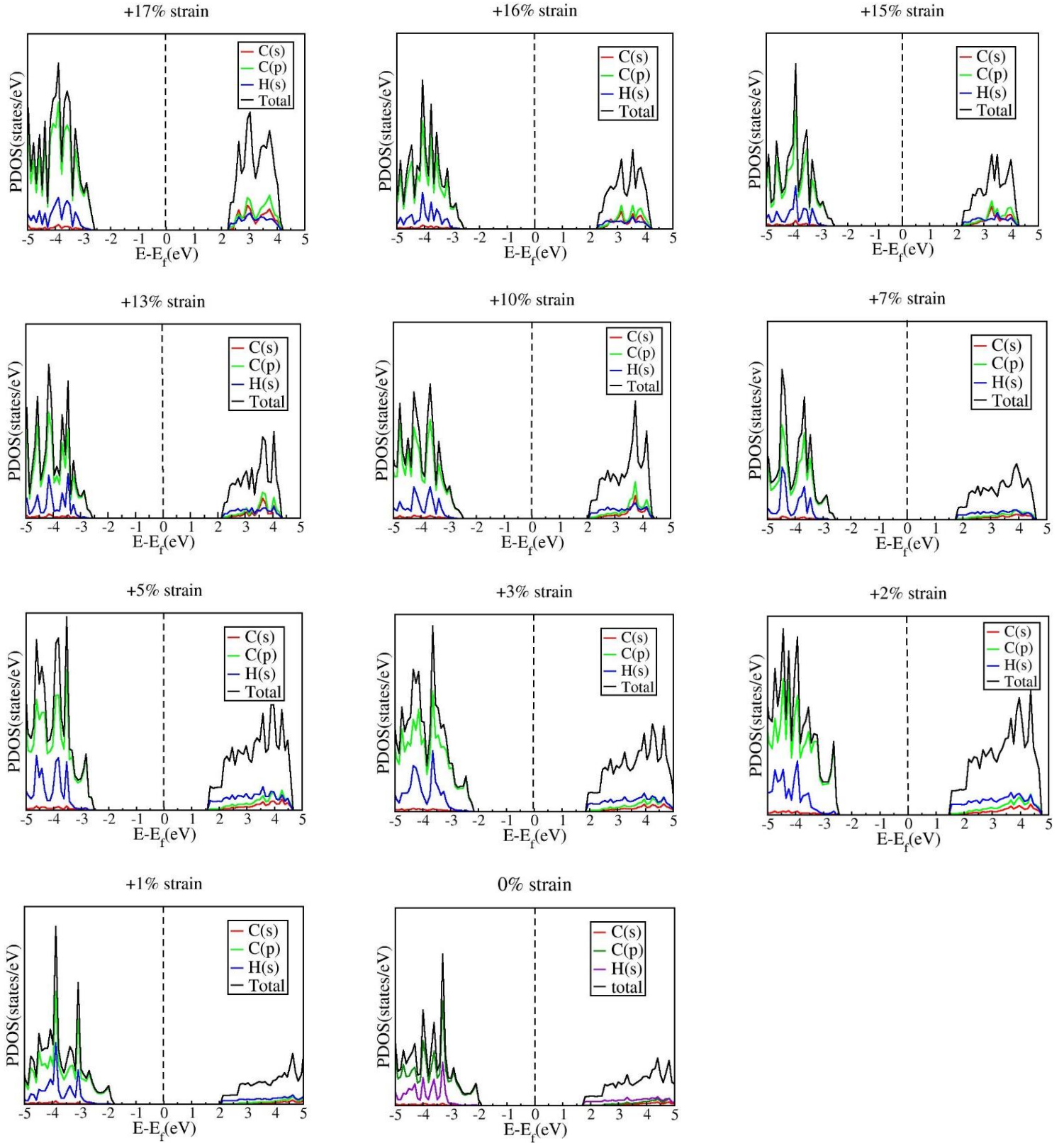


Figure S12: PDOS of ψ -graphane at different values of positive strain.

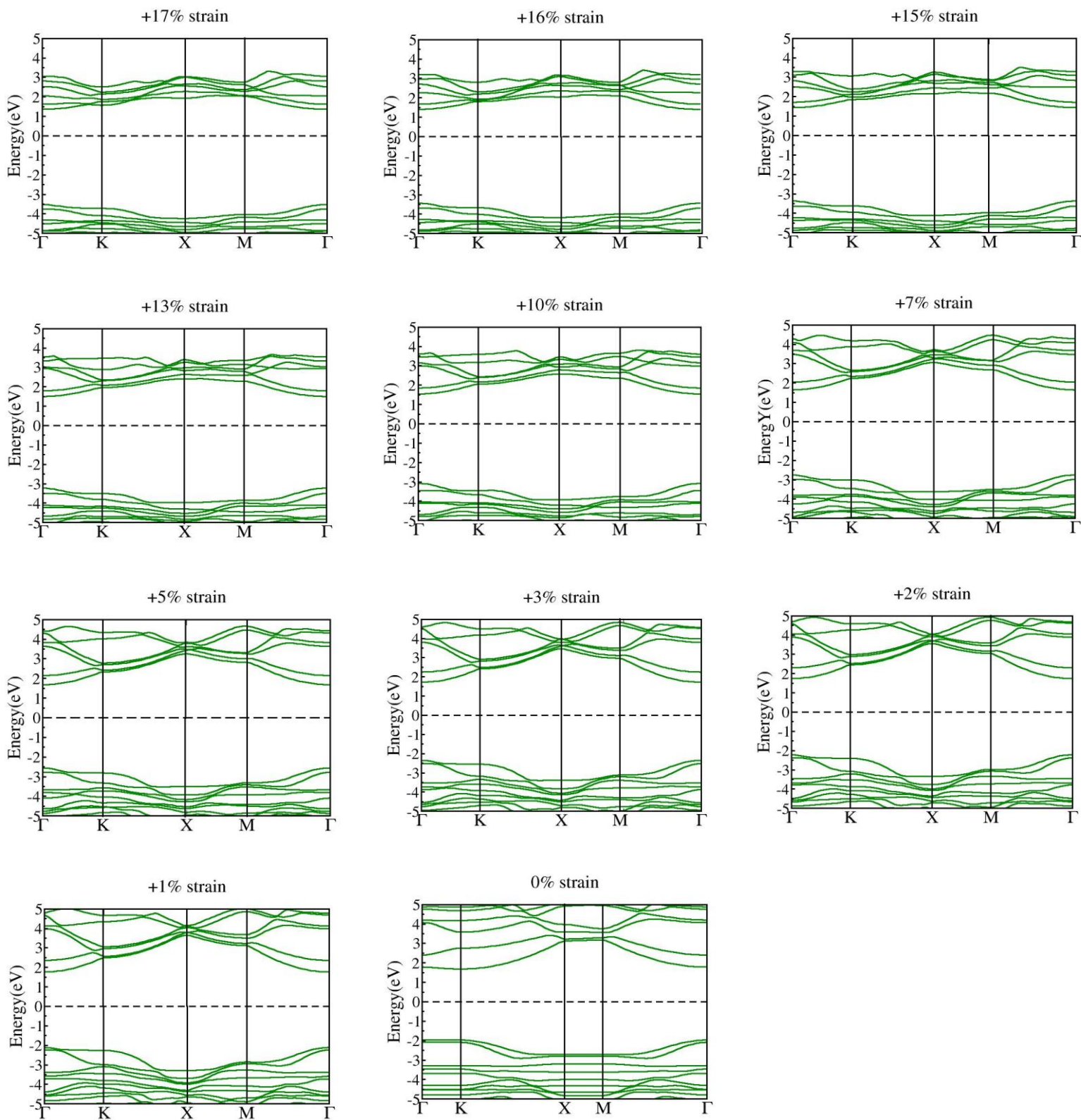


Figure S13: Electronic band structure of ψ -graphane at different values of positive strain.

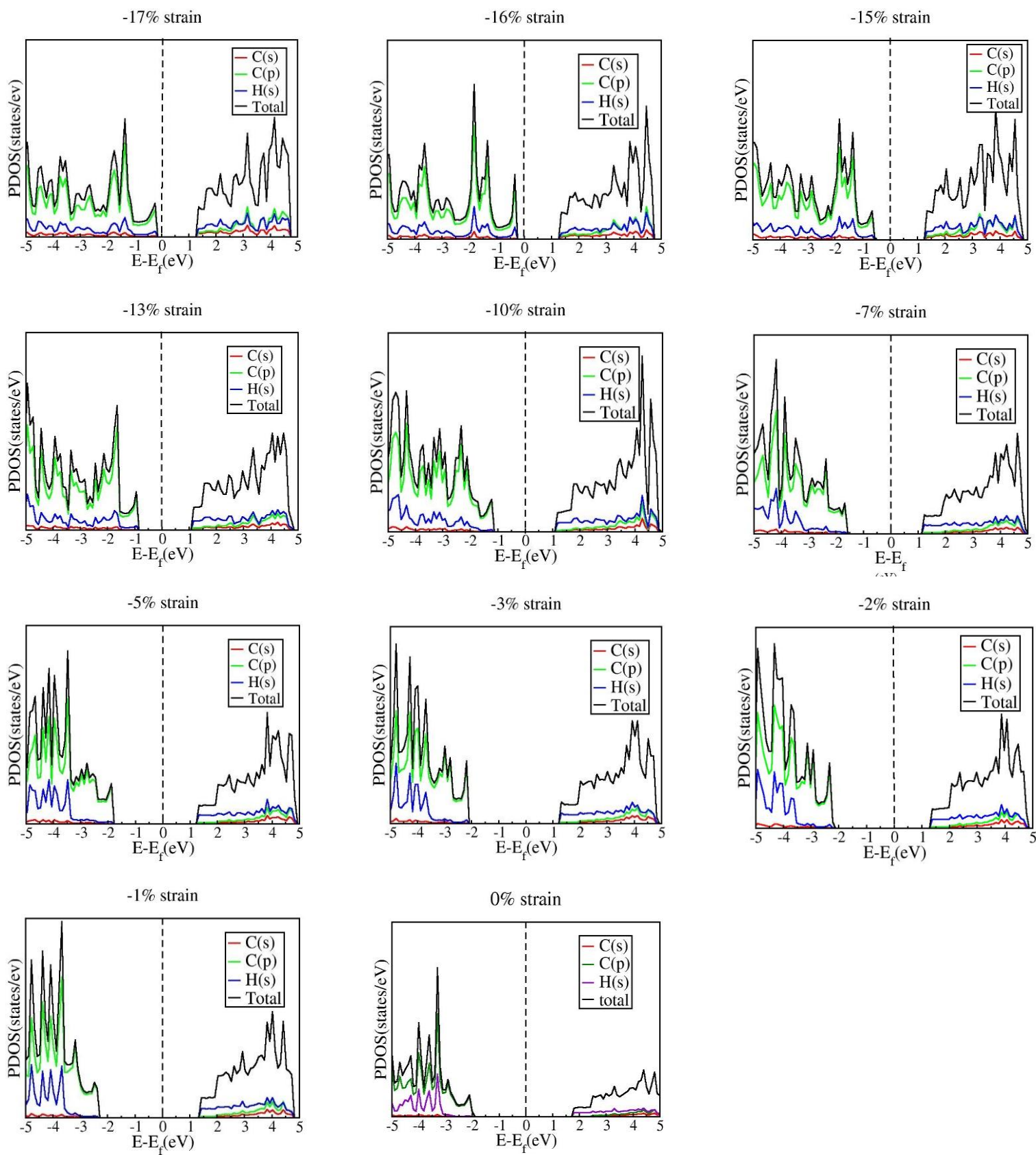


Figure S14: PDOS of ψ -graphane at different values of negative strain.

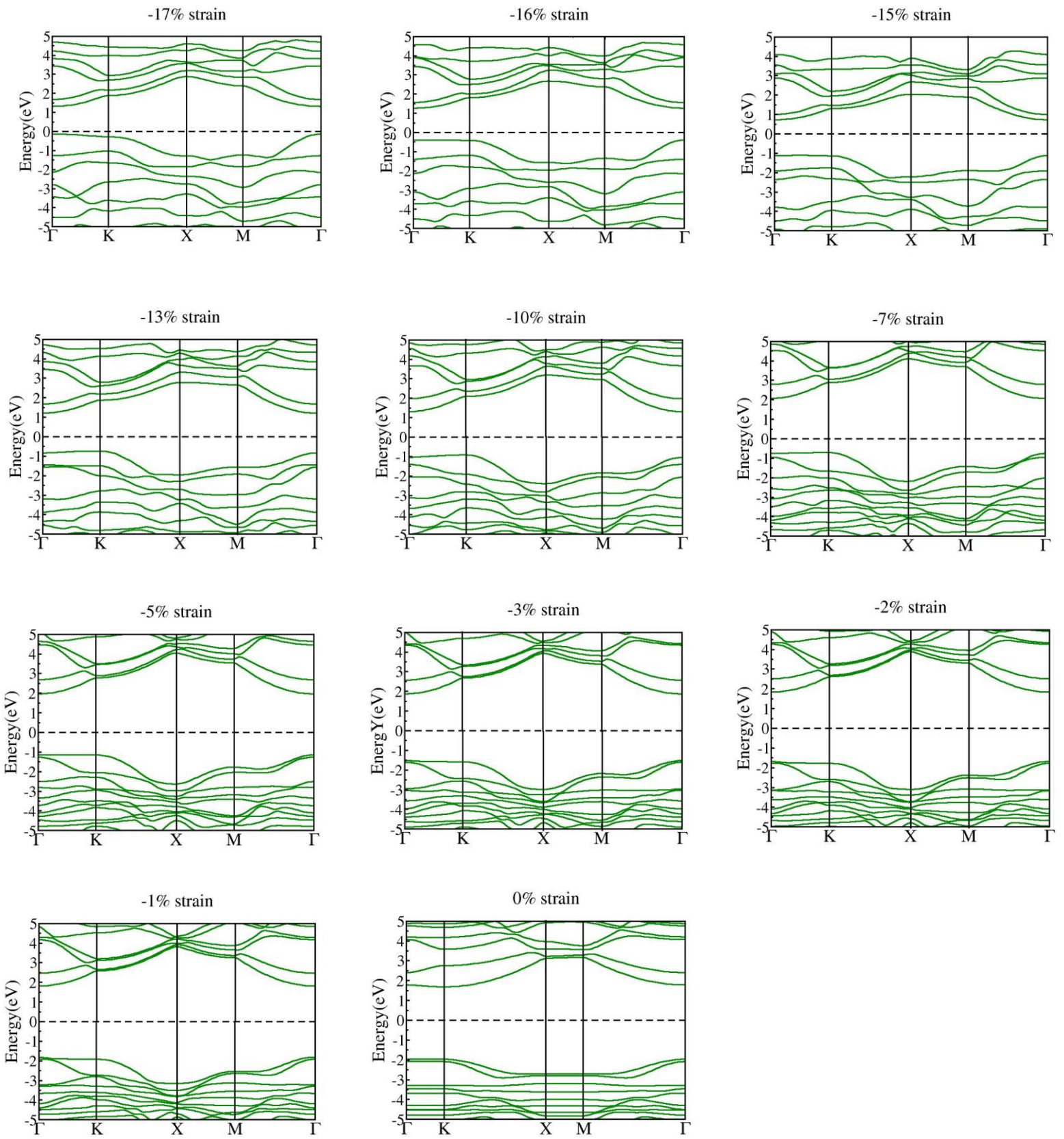


Figure S15: Electronic band structure of ψ -graphane at different values of negative strain.

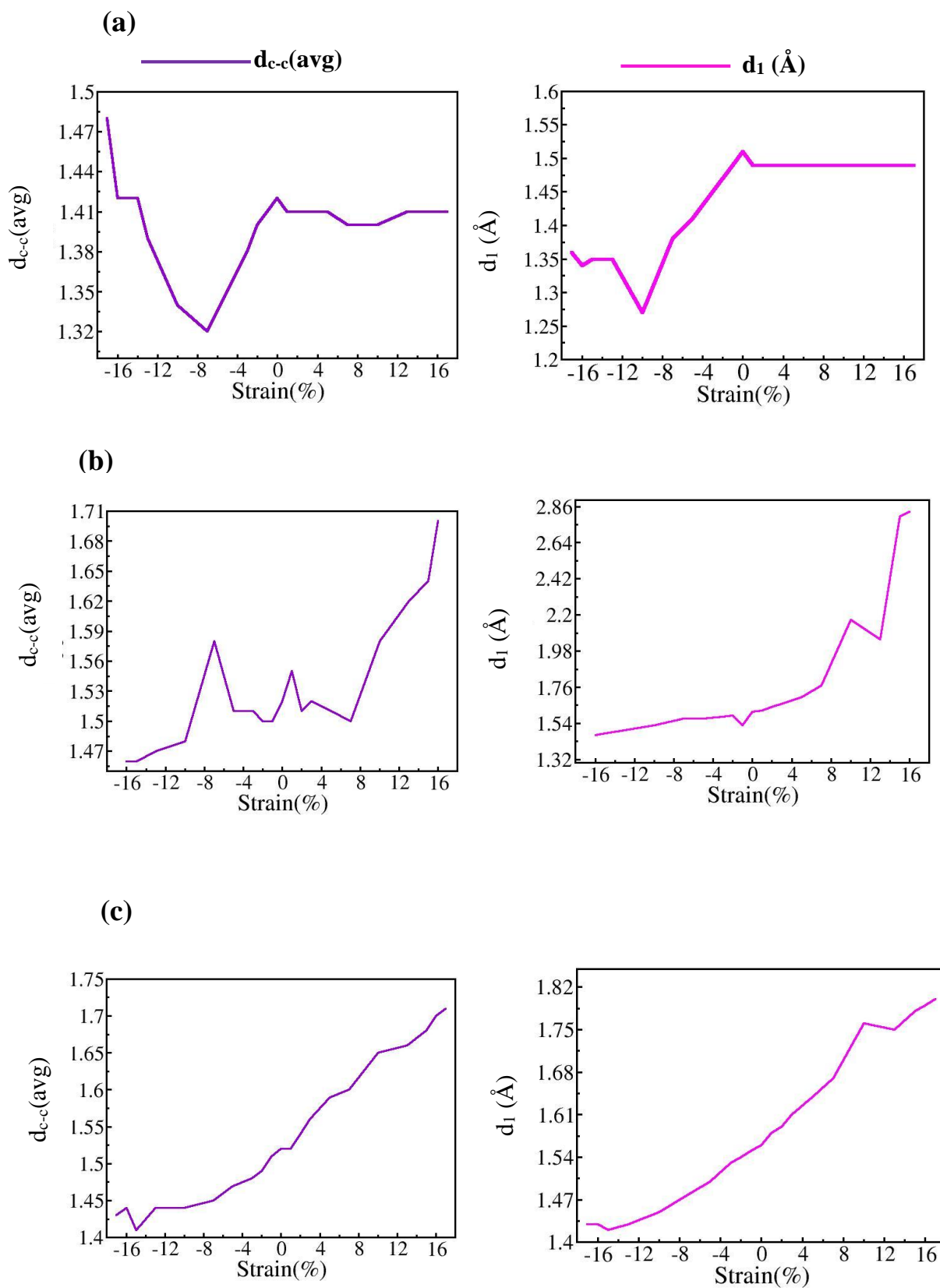


Figure S16: Variation of average bond lengths d_{c-c} (avg) (left) and d_1 (Å) (right) with applied uniform biaxial mechanical strain in (a) ψ -graphene, (b) ψ -graphone and (c) ψ -graphane.