

Supporting Information

for

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

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Additional figures

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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.



+16% strain

+15% strain

+17% strain

4

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 -graphone at different strain values.



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



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



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



Figure S10: Electronic band structure of ψ -graphone 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.