

Supporting Information to:

Charge-induced electromechanical actuation of two-dimensional hexagonal and pentagonal materials

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2. Methodology

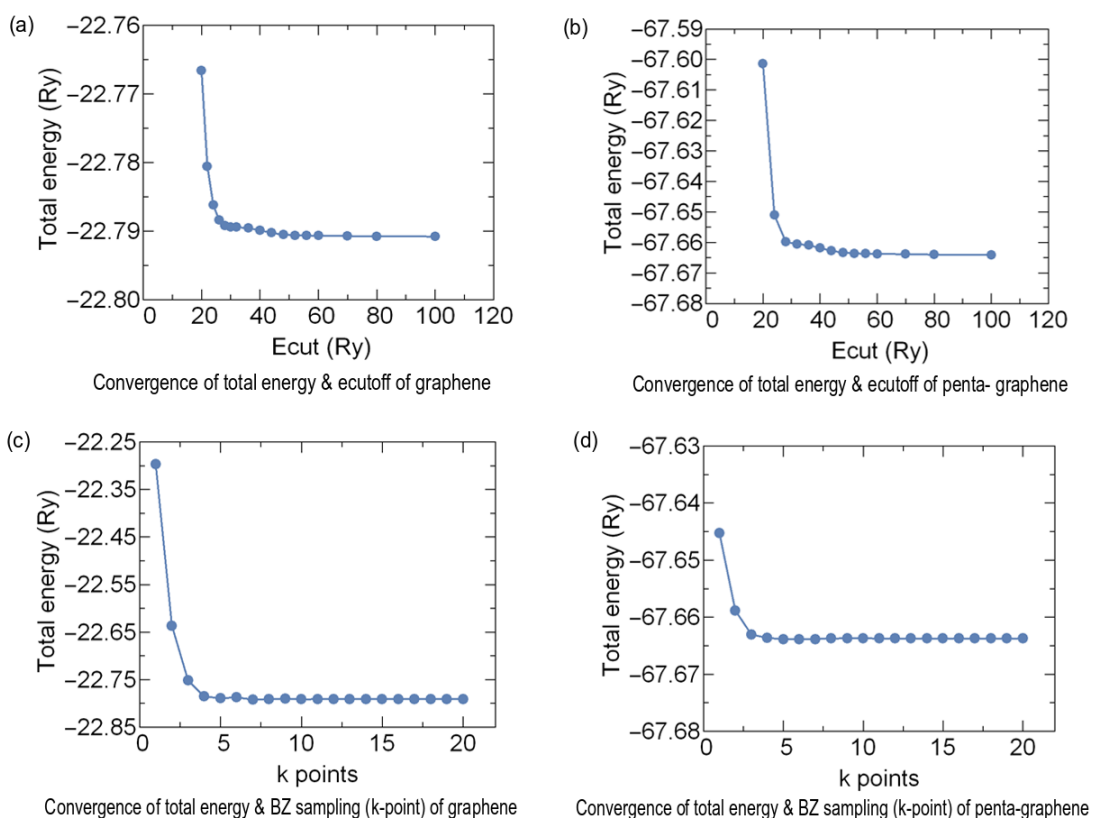


Fig. S1. Convergence of total energy and energy-cutoff of (a) graphene and (b) penta-graphene. Convergence of total energy and grid size (k-point) of (c) graphene and (d) penta-graphene.

3. Results and discussion

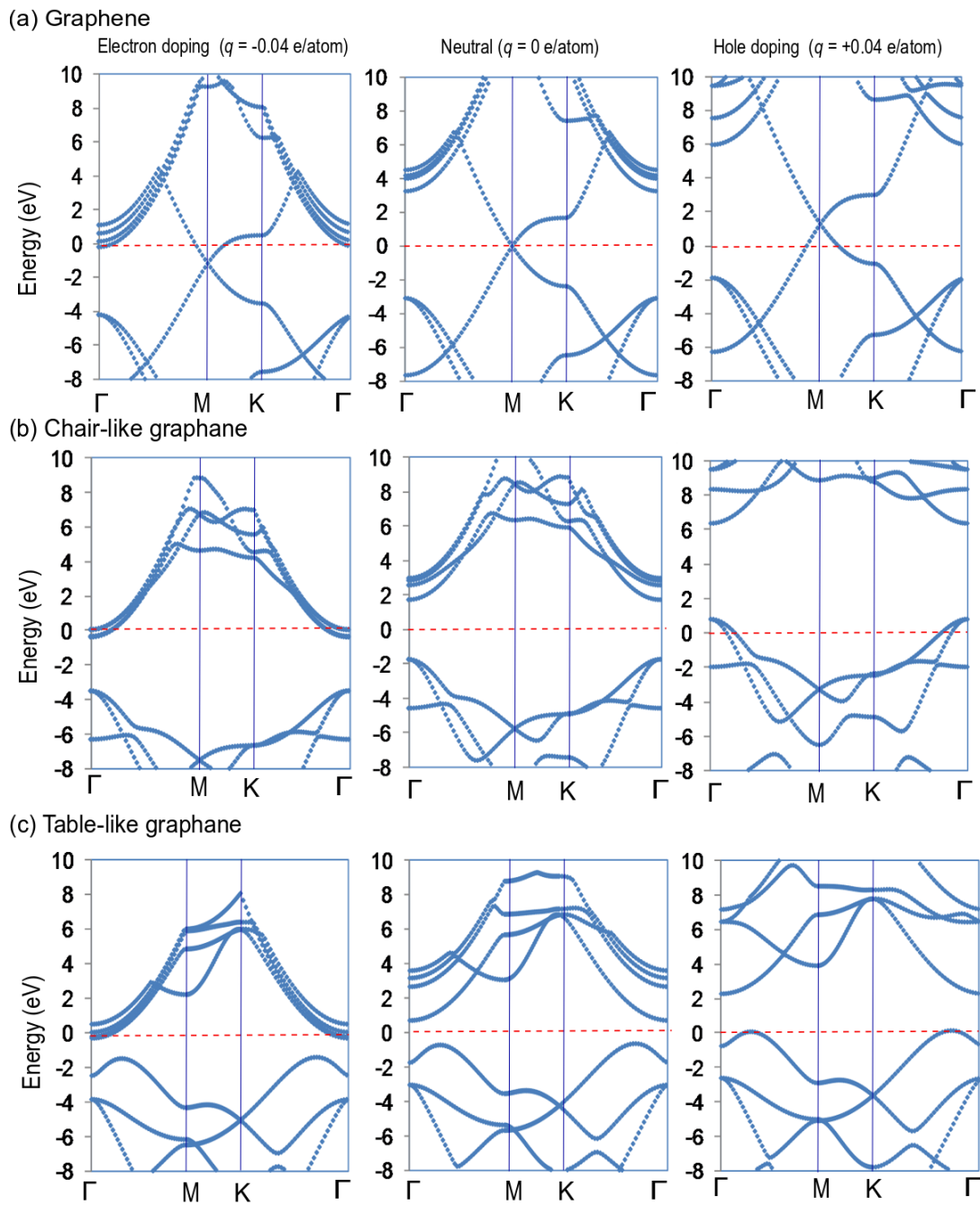


Fig. S2. Band structure of 2D materials: (a) graphene, (b) chair-like graphane and (c) table-like graphane. The Fermi energy (dashed line) is set to zero for all plots.

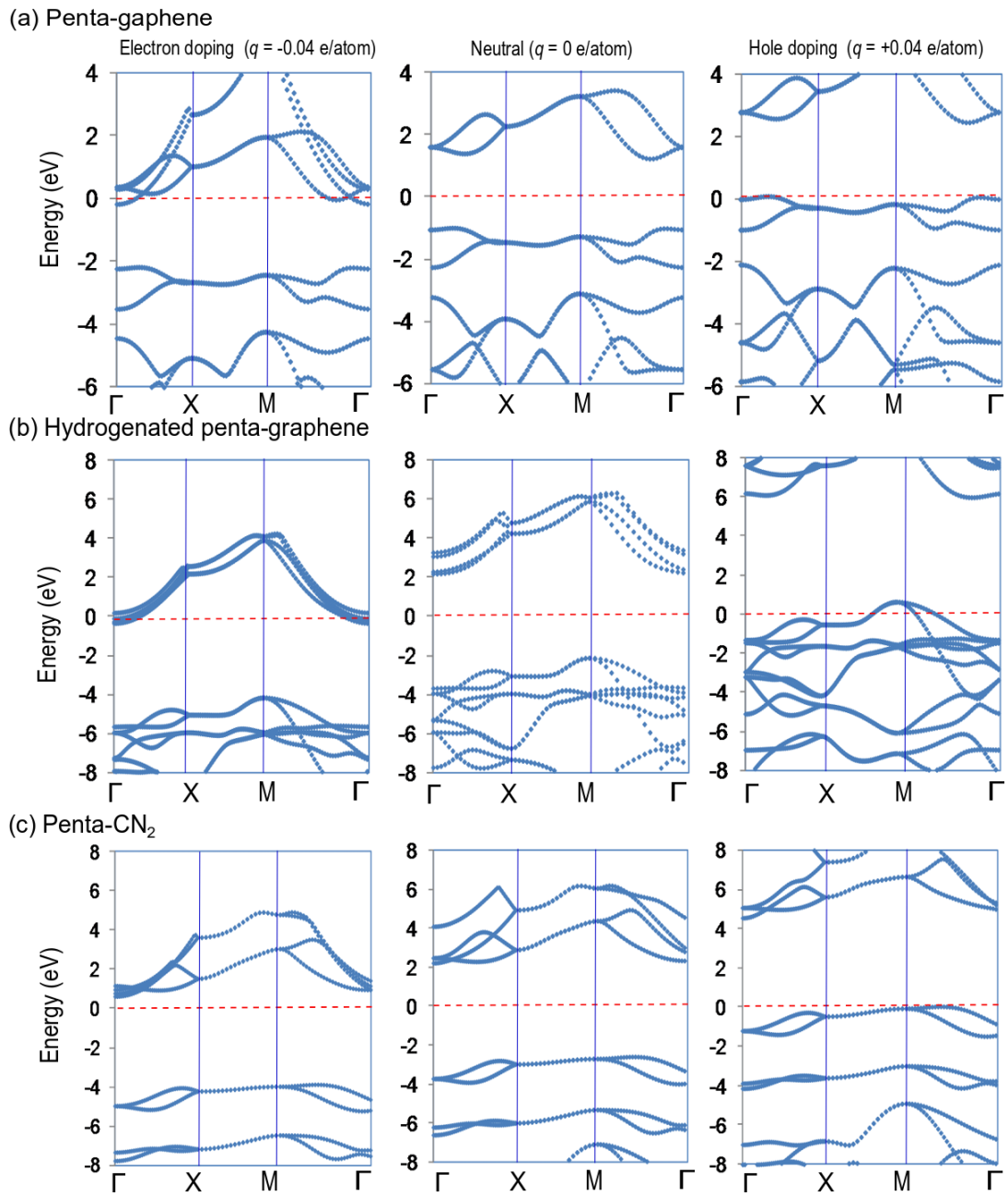


Fig. S3. Band structure of 2D materials: (a) penta-graphene; (b) hydrogenated penta-graphene and (c) penta-CN₂. The Fermi energy (dashed line) is set to zero for all plots.