Influence of Single-Vacancy Defect Arrangement on Graphene Electronic Structure

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Defect engineering provides a powerful route for tuning the electronic properties of graphene. Building on previous tight-binding studies of periodically arranged single-vacancy (SV) defects [1], we perform density functional theory (DFT) calculations to investigate the influence of SV sublattice configuration and directional spacing on graphene's electronic structure. Our results confirm that SV defects located on the same sublattice exhibit predictable electronic behaviour, following trends similar to armchair graphene nanoribbons (AGNRs) for dispersive bands, in addition to low-dispersion bands originating from unpaired states due to the sublattice imbalance. Notably, these effects are largely independent of defect density, with sublattice configuration remaining the dominant. Overall, our DFT results validate previous tight-binding predictions and demonstrate that the relative arrangement of SV defects constitutes an additional degree of freedom for electronic structure engineering in graphene. Importantly, our findings show that the electronic structure remains systematically tuneable despite the presence of defects.

References

[1] AIP Advances 16(1) (2026) 015307

Figures

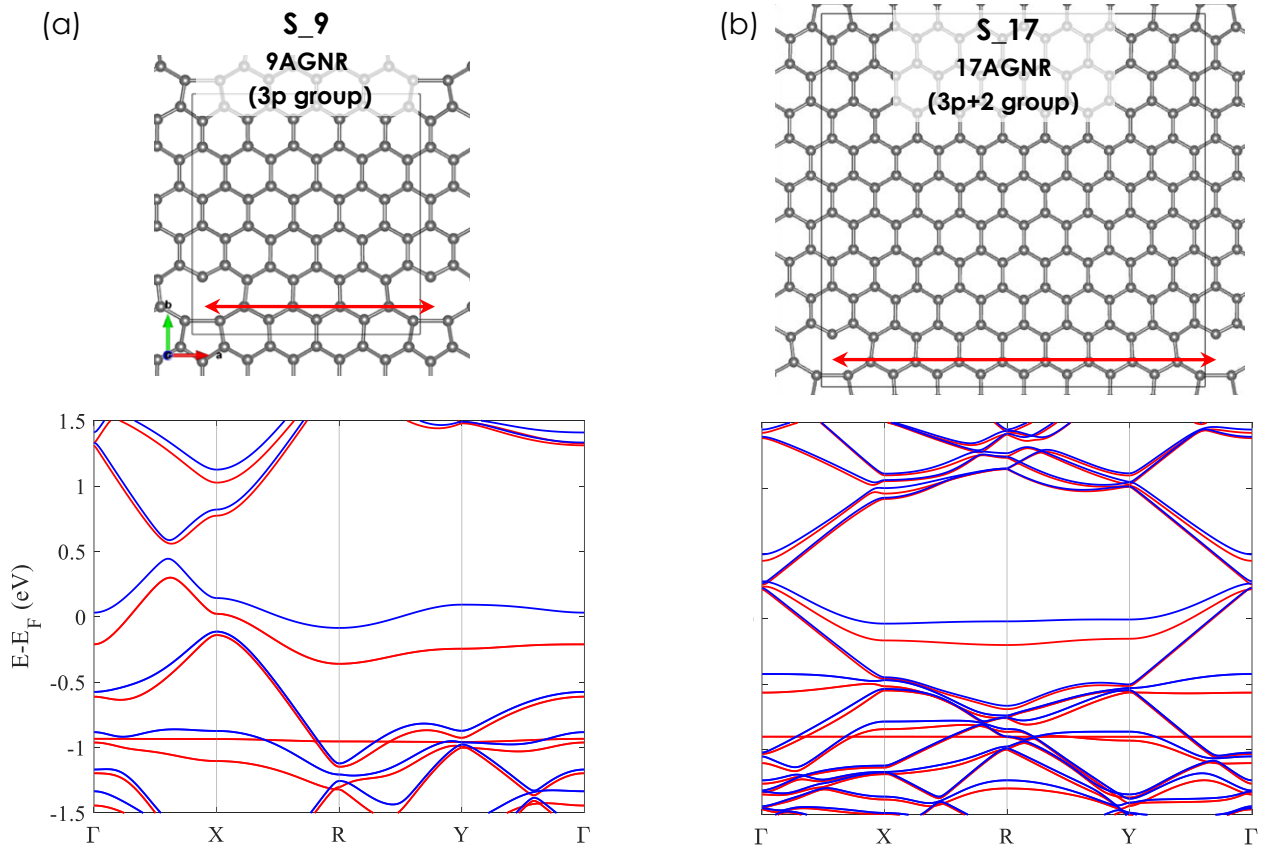

Figure 1: (a) Atomic structure (up) and band structure (down) for an SV defected system with 9 atoms spacing (S_9). (b) Similar to (a) for S_17.