Supporting Information

Coronene based Graphene Nanoribbons Insulated by Boron Nitride Nanotubes; towards Electronic Properties of the Hybrid Structure

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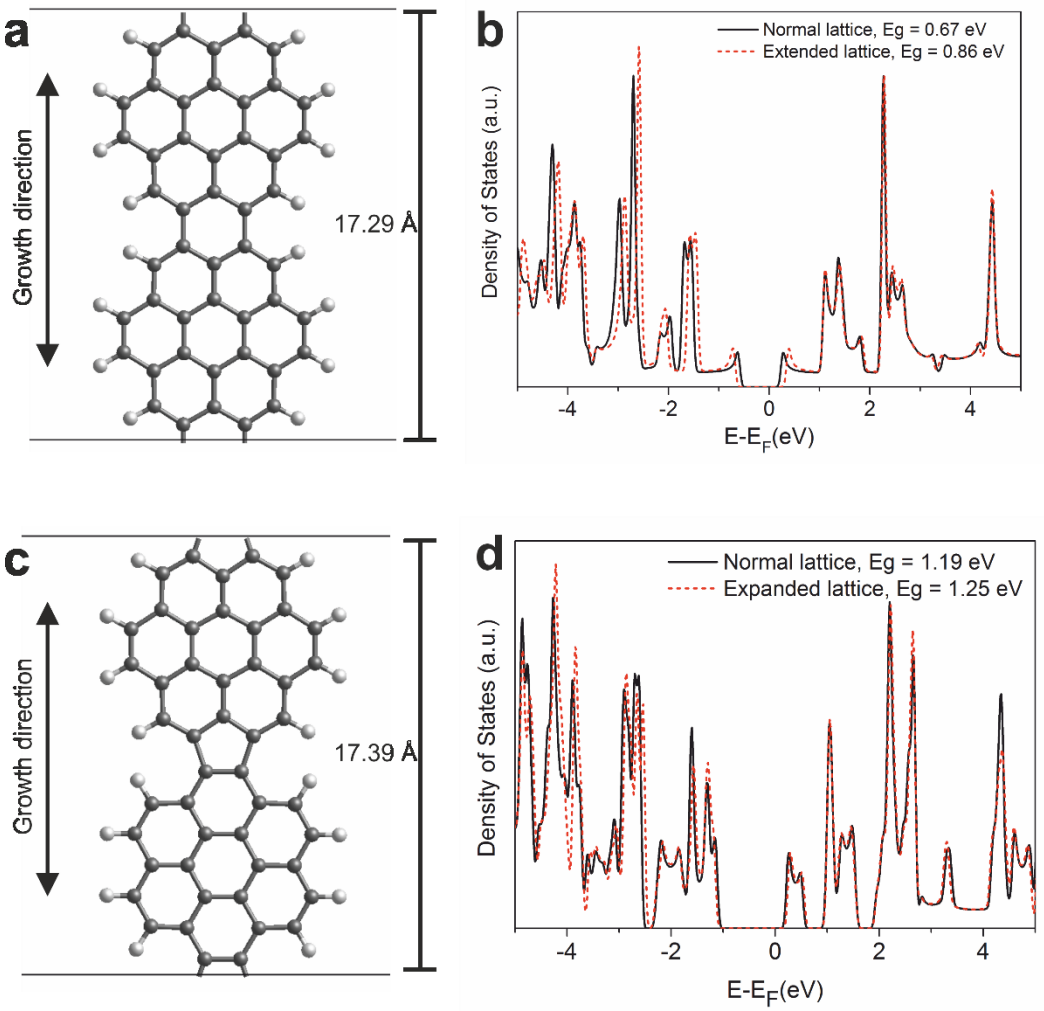

Figure S1. Coronene-based 7-GNR. (a) The super cell consist of two coronene molecules with a lattice parameter along the growth direction of 17.29 Å. (b) Density of States (DOS) of the 7-GNR at the equilibrium lattice parameter (17.29 Å) and at expanded lattice of 17.56 Å. (c) Defective 12-GNR. (d) DOS at the equilibrium lattice parameter of 17.39 and at the expanded lattice of 17.56 Å.

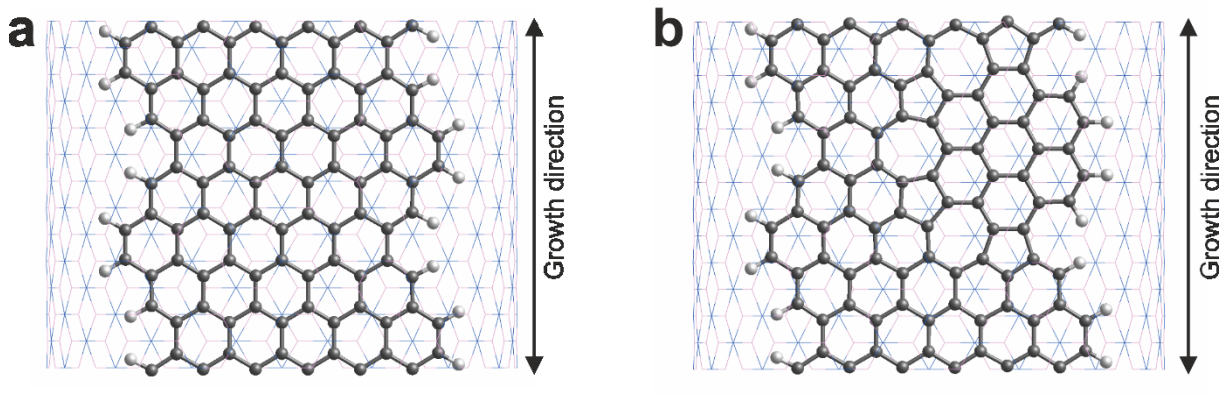

Figure S2. Optimized geometry of (a) pristine and (b) defective 12-GNR encapsulated inside a (16,16)-BNNT. The lattice parameter is 17.56 Å for both systems.

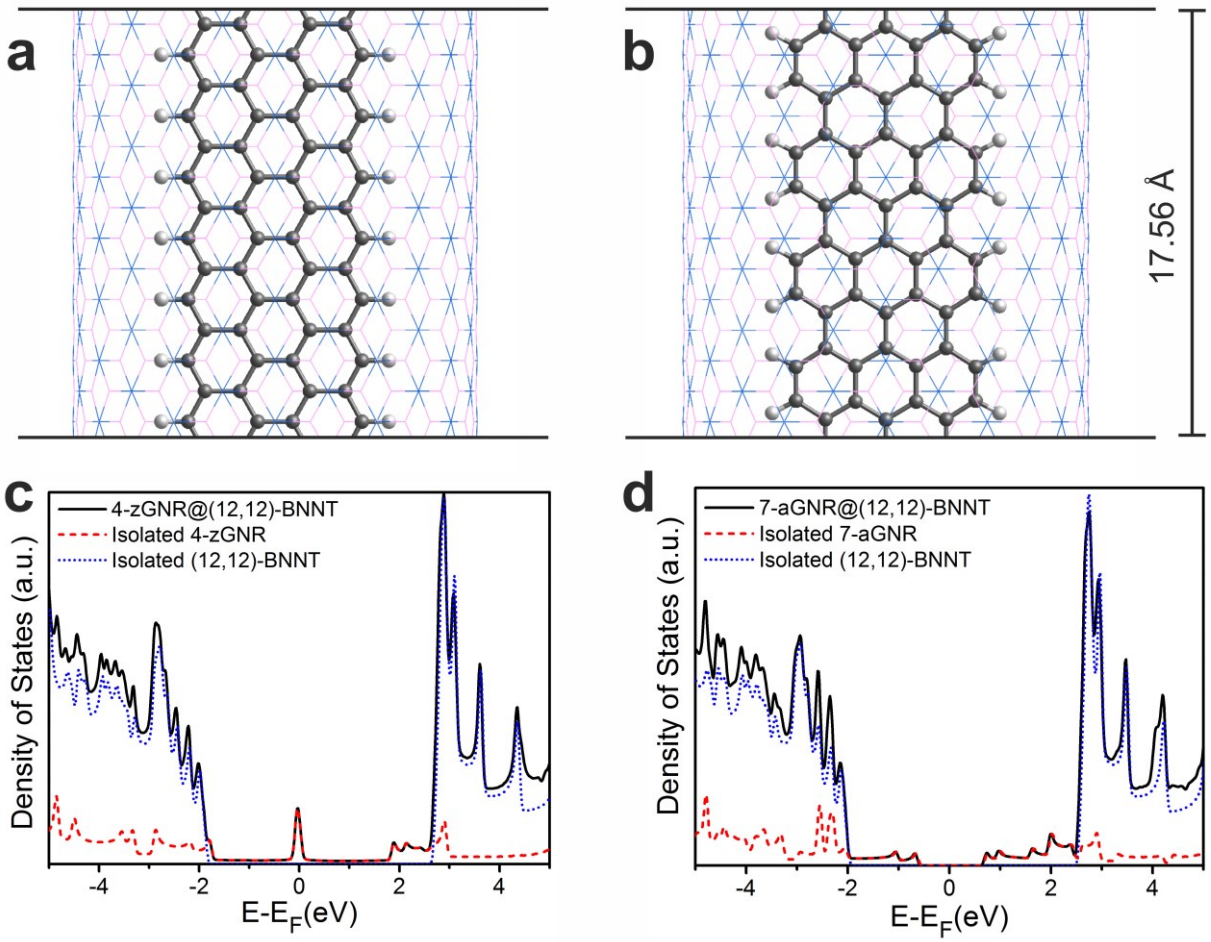

Figure S3. Optimized structure of (a) 4-zigzag (4-zGNR) and (b) 7-armchair (7-aGNR) graphene nanoribbons inside a (12,12)-BNNT. (c-d) Density of states of the isolated and composite systems.

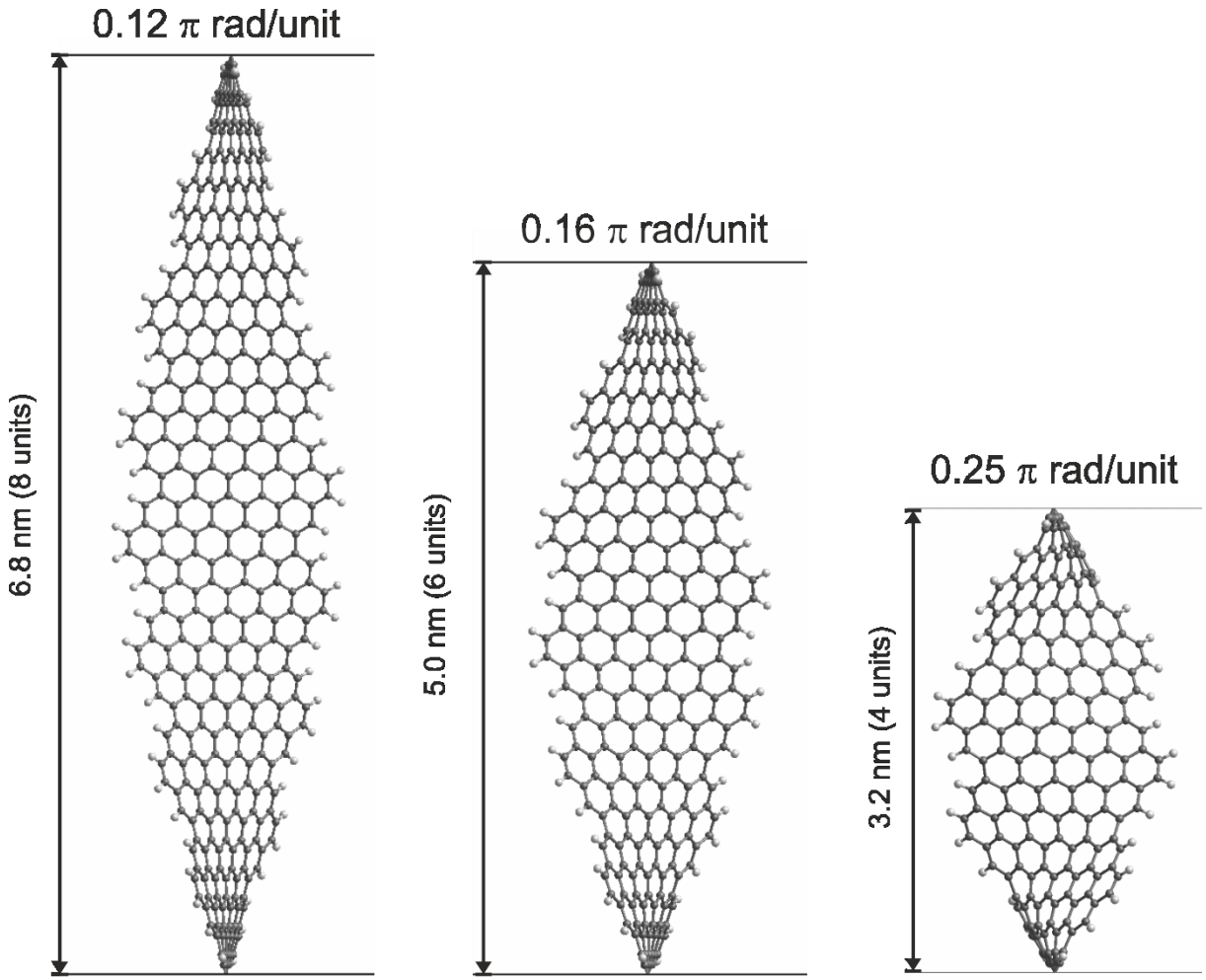

Figure S4. Optimized geometries of non-defective 12-GNR at different twisting rates. The distance indicates the necessary length to achieve a half-turn, and the units specify the number of unit cells in each system. Similar configurations are observed for the 7-GNRs as well as the defective systems.

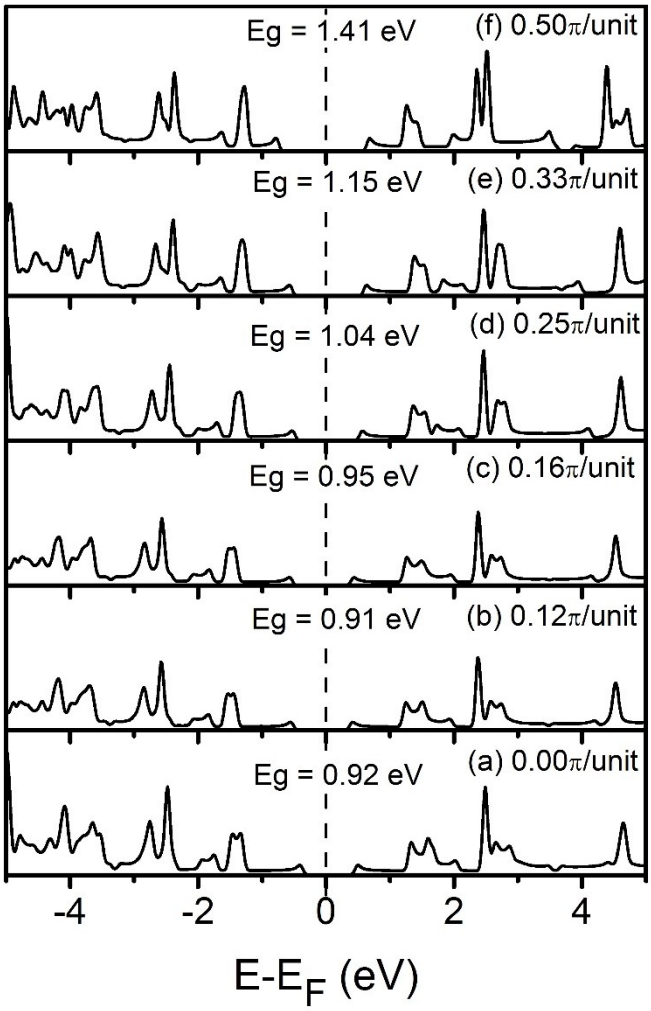

Figure S5. DOS of 7-GNR at different twisting rates.

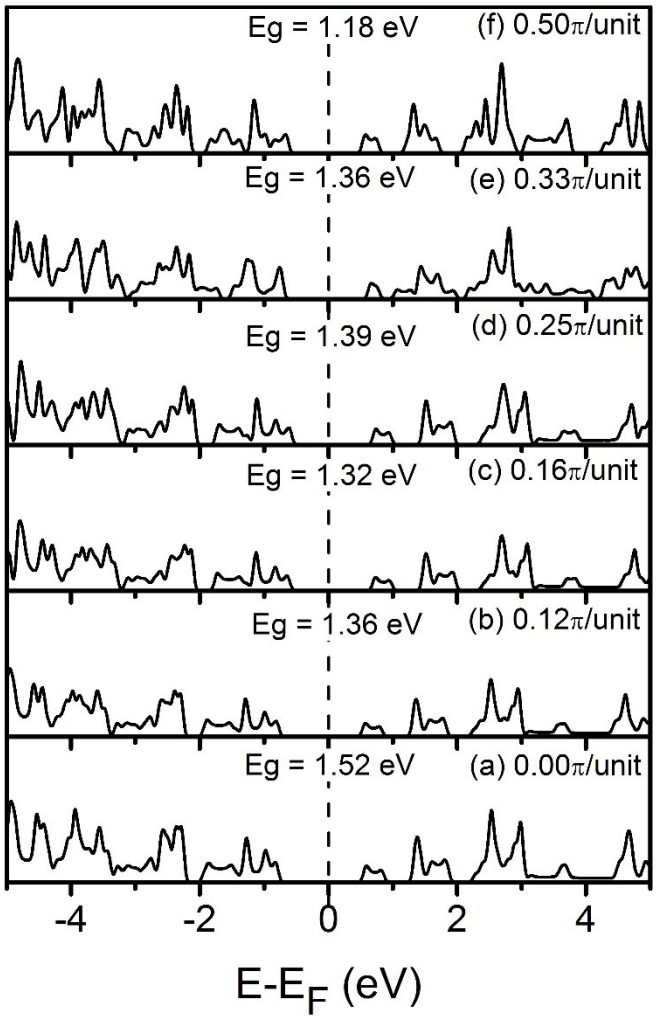

Figure S6. DOS of defective 7-GNR at different twisting rates.

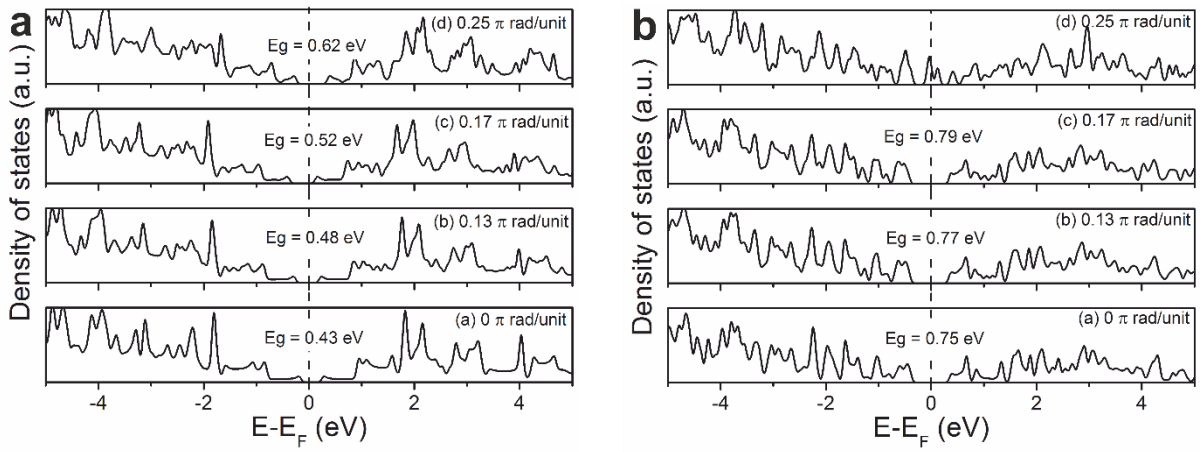

Figure S7. DOS of (a) non-defective and (b) defective 12-GNRs at different twisting rates.

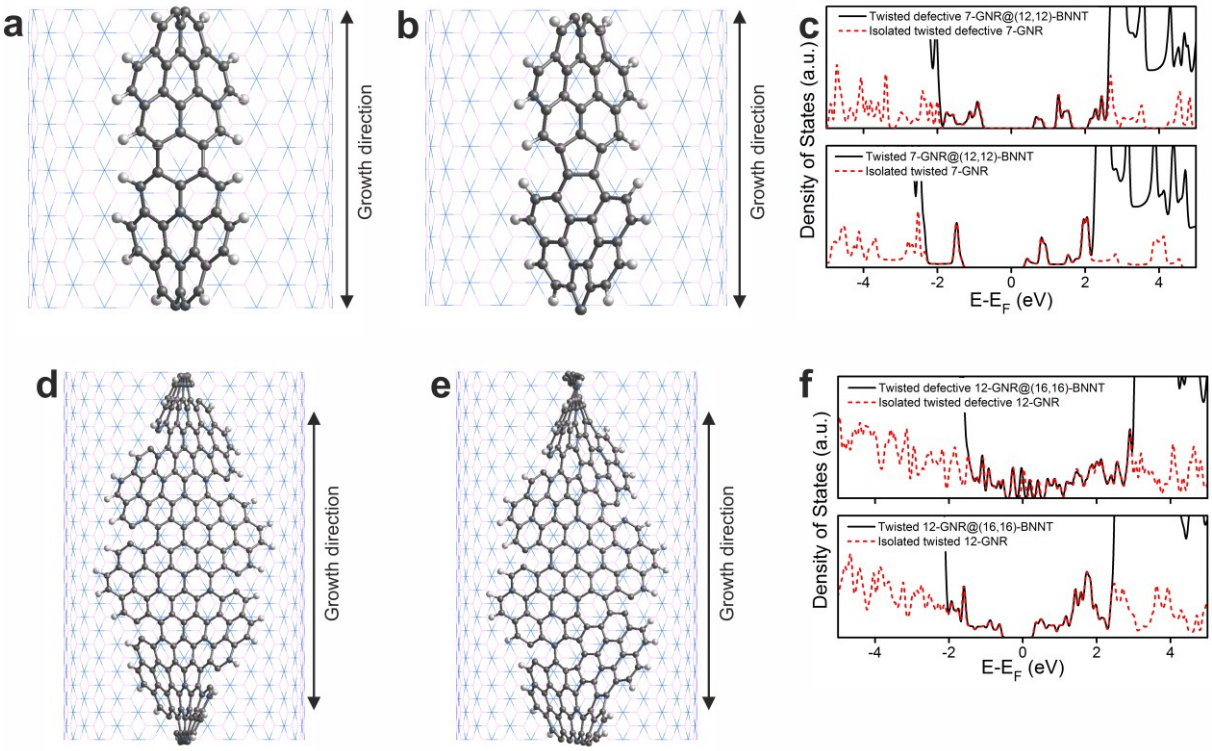

Figure S8. Optimized geometries of (a) non-defective and (b) defective 7-GNR@(12,12)-BNNT twisted at 0.50π rad/unit, and their respective (c) density of states. The lattice parameter for both systems is 17.56 Å. Optimized geometries of (d) non-defective and (e) defective 12-GNR@(16,16)-BNNT twisted at 0.25π rad/unit with their respective (f) density of states. The lattice parameter for both systems is 35.12 Å.

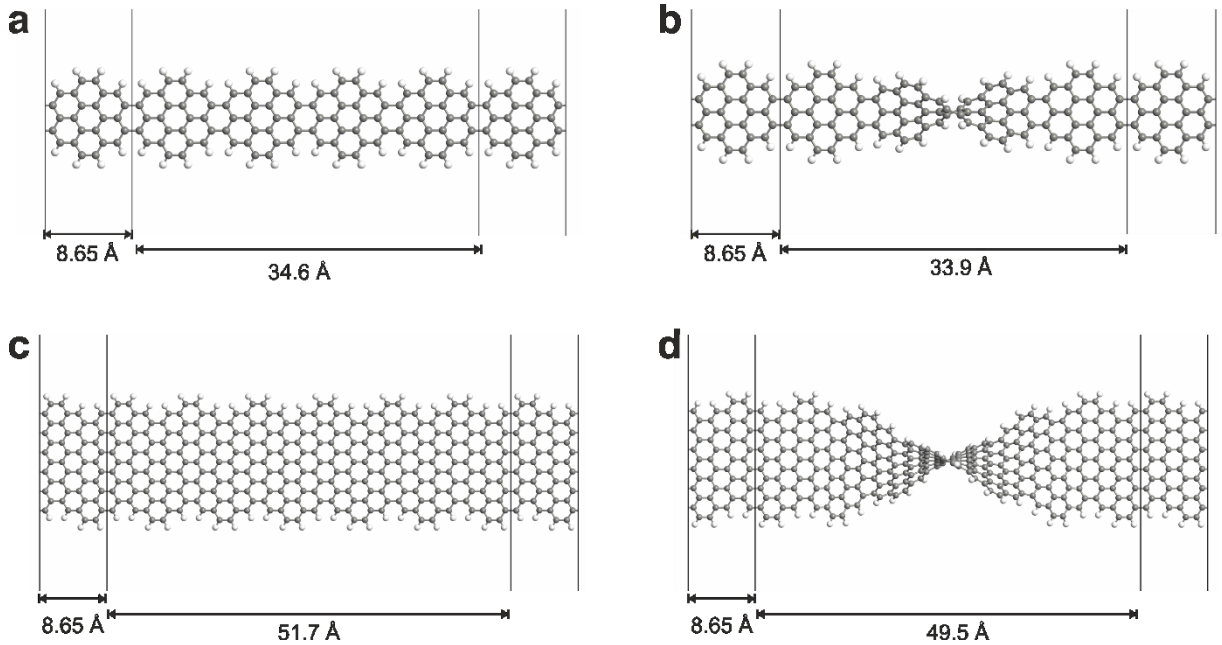

Figure S9. Device configuration used to calculate the electron transport properties for (a) Planar 7-GNR, (b) twisted 7-GNR, (c) planar 12-GNRs and (d) twisted 12-GNR. Similar device configurations are used for defective 7- and 12-GNRs.