

Auxiliary Materials for
Deriving carbon atomic chains from graphene

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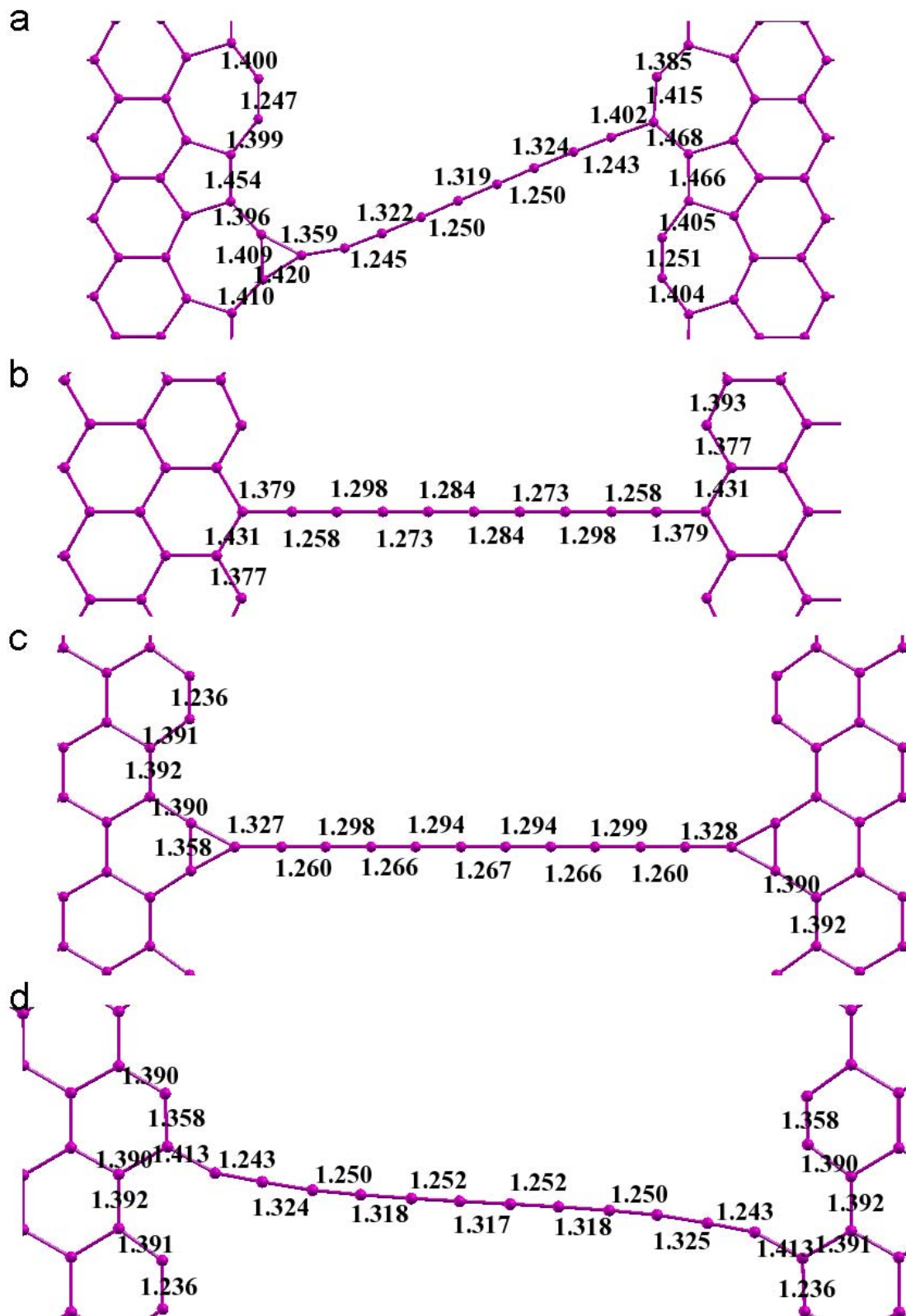


FIG. S1. Optimized geometries of carbon atomic chains constrained by two GNRs with various types of edges. (a) a 8-sp-atom chain bridging two GNRs with 5-7 edges,

(b) a 9-sp-atom chain bridging two GNRs with zigzag edges, (c) a 10-sp-atom chain bridging two GNRs with armchair edges, (d) a 12-sp-atom chain bridging two GNRs with armchair edges. The unit for bond length is Å.

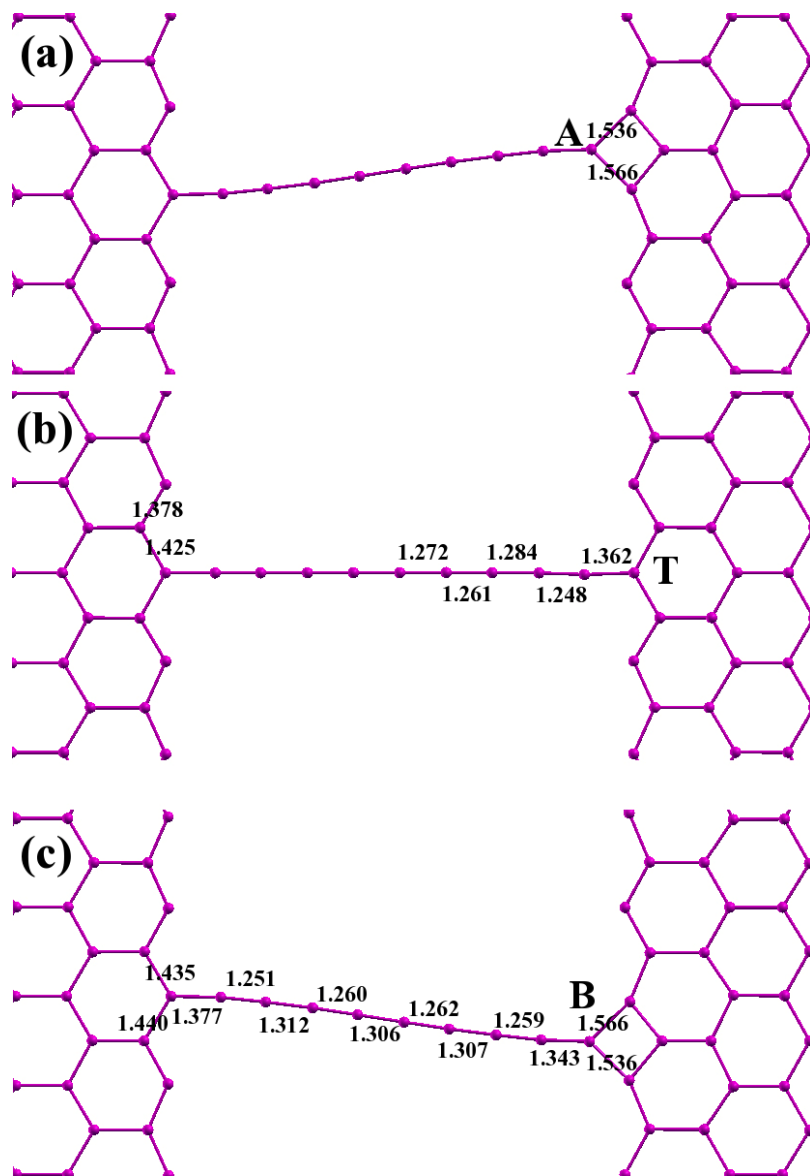


FIG. S2. One of the possible pathways for the migration of a 3% strained carbon chain along the graphene with zigzag edge. (a) Initial state, (b) transition state, (c) final state. The unit for bond length is Å.