

## Supplementary Material for

Article

# Insertion of the Liquid Crystal 5CB into Monovacancy Graphene

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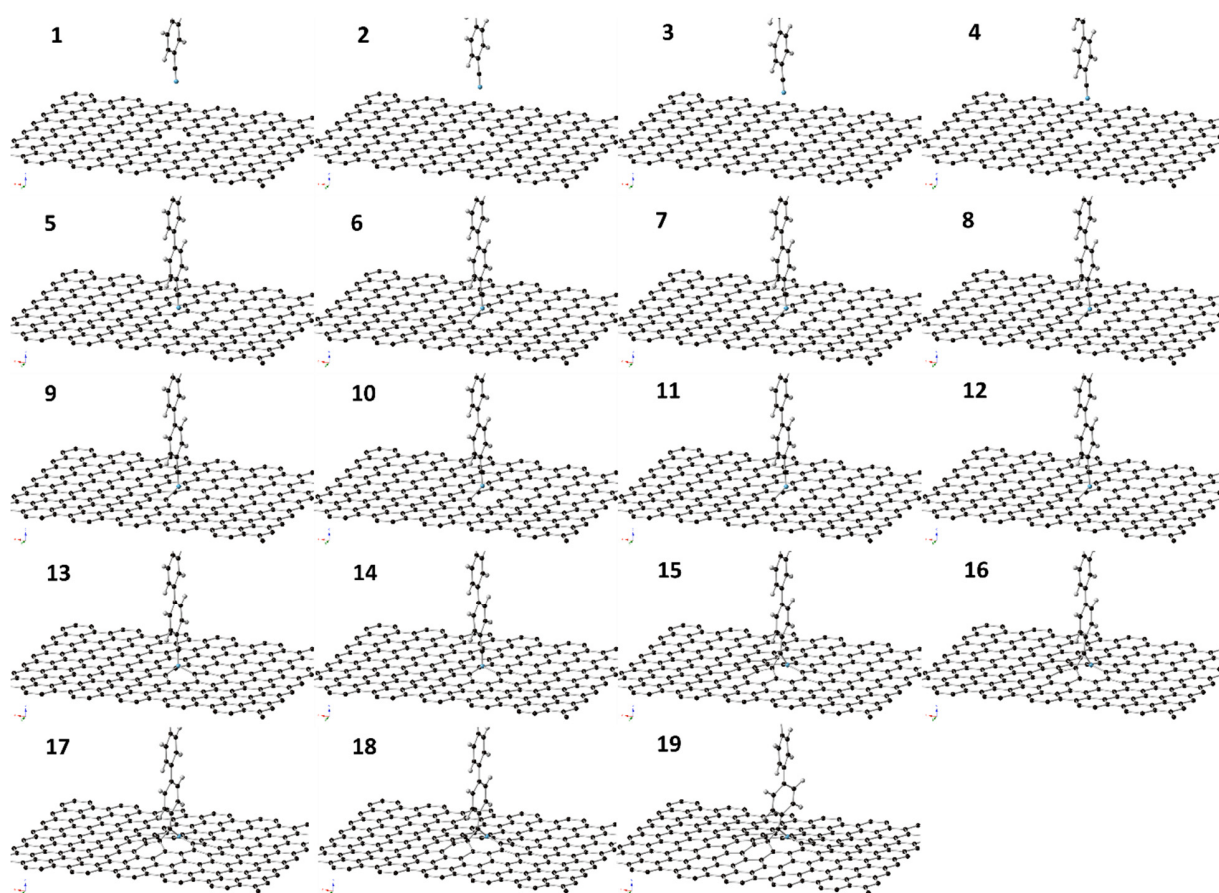


Figure S1. Atomic structures for the 19 reaction steps generated by the nudge elastic band method for the process of chemical insertion of 4-cyan-4'-pentylbiphenyl (5CB) into a graphene monovacancy.

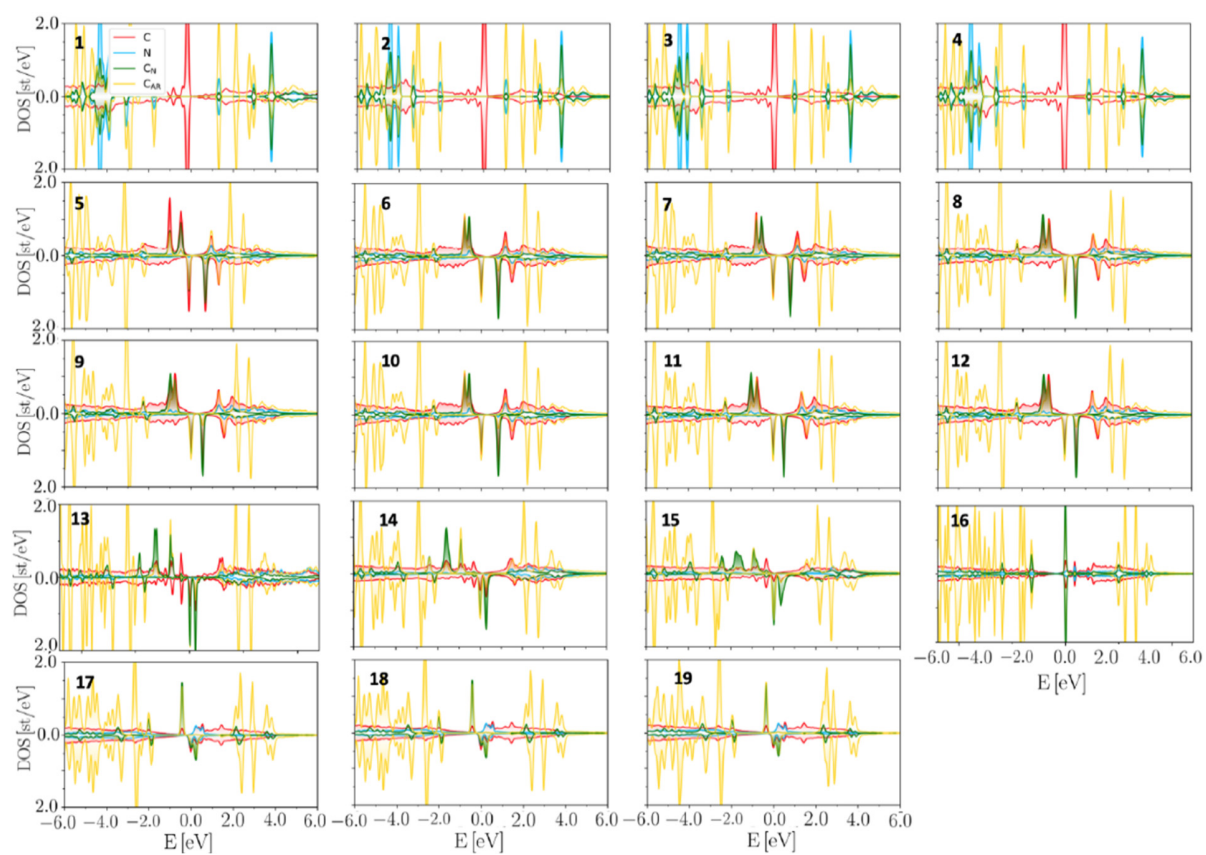


Figure S2. The partial densities of states (PDOS) for the 19 reaction steps generated by the nudge elastic band (NEB) method for the process of 4-cyan-4'-pentylbiphenyl (5CB) into a graphene monovacancy.