Emergent Properties and Trends of a New Class of Carbon Nanocomposites: Graphene Nanoribbons Encapsulated in a Carbon Nanotube

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Supporting Information:

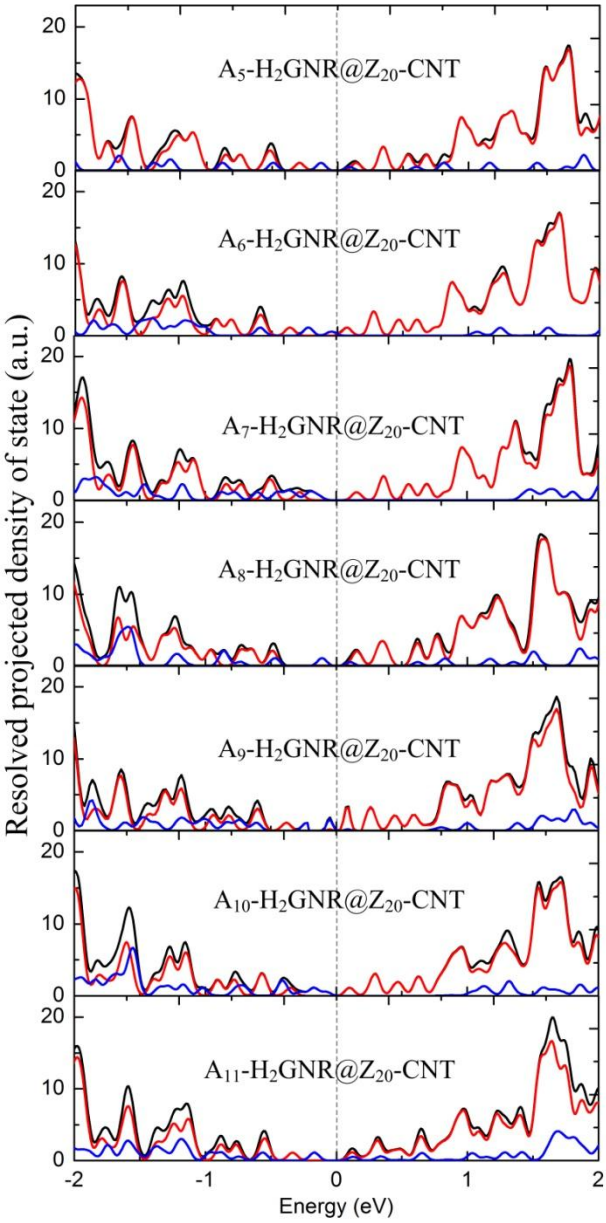

Figure S1. Resolved density of states for all A_n-H_2GNR@Z_{20}-CNT. The black lines are for total DOS, the red (blue) lines are for DOS from CNT (GNR).

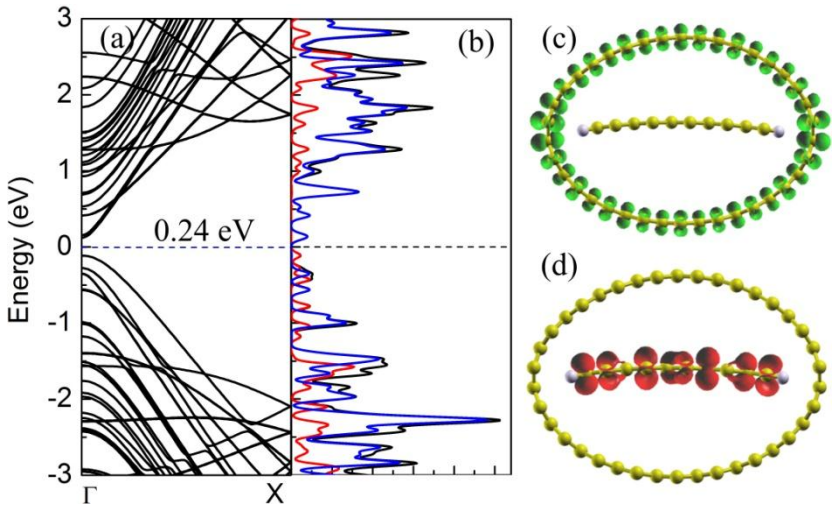

Figure S2. Band structures (a) and corresponding resolved density of states (b) for A_{10}-H_2GNR@Z_{19}-CNT. The wavefunction spatial distributions of CBM (c) and VBM (d) are also presented.

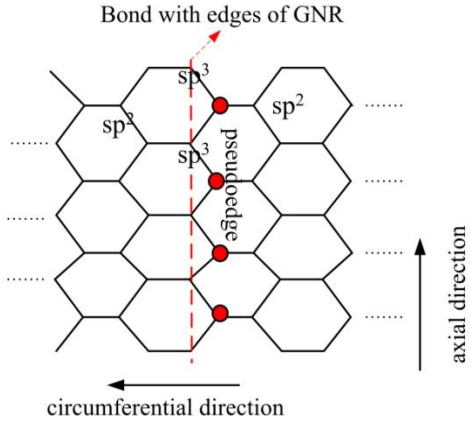

Figure S3. Illustration of part of the wall of armchair CNT after bonding with the edges of a zigzag GNR (red dashed line). A pseudo-edge is formed as indicated.

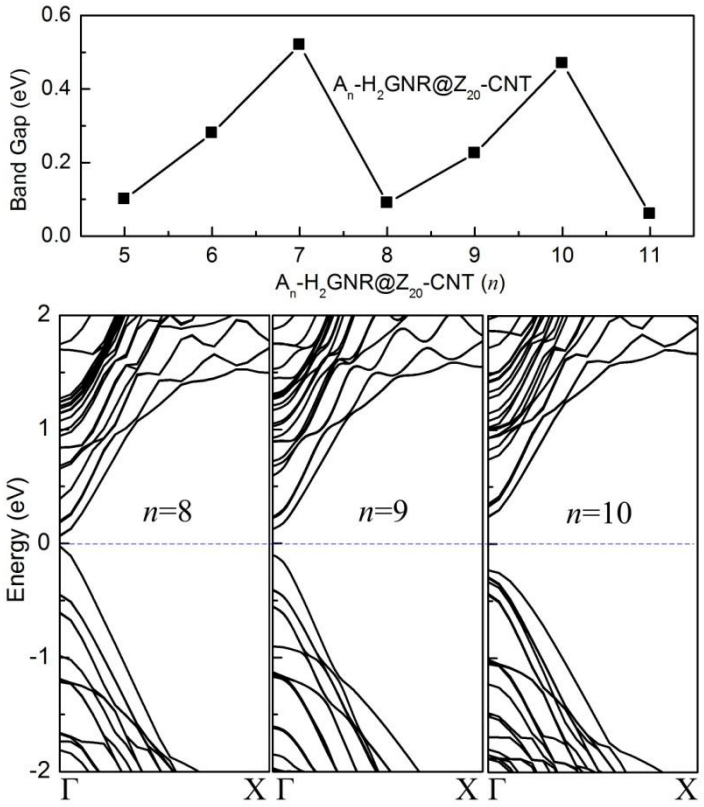

Figure S4. Band gap variation of An-H2GNR@Z20-CNT as a function of the width of encapsulated GNRs (above). Band structures for An-H2GNR@Z20-CNT with n= (below left) 8, (below center) 9, (below right) 10. The calculations were performed using ab-initio density functional theory in conjunction with all-electron projector augmented wave potential, and the Perdew-Burke-Ernzerhof generalized gradient approximation (GGA) to the electronic exchange and correction, as implemented in VASP. The other parameters of calculations are the same as those in SIESTA, except the introduction of vdWs. We incorporate the vdWs interactions by adding a semi-empirical dispersion potential to conventional KS DFT energy, through a pair-wise force field following Grimme's DFT-D2 method.