Supporting information for

Excitons of edge and surface functionalized graphene nanoribbons

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Figure Captions

Figure S1: PDOS of $P_z$ of carbon and fluorine and 1s of hydrogen of H-W9-H (a), F-W9-H (b), F-W9-F (c), H-W10-H (d), F-W10-H (e), F-W10-F (f). For instance, “edge C(F)” means the PDOS of $P_z$ of C atoms at the edges connected with F atoms; “edge C(H)” means the PDOS of $P_z$ of C atoms at the edges connected with H atoms; “Total C” means the PDOS of $P_z$ of all the C atoms; “F” means the PDOS of $P_z$ of F atoms at the edges; and “H” means the PDOS of 1s of H atoms at the edges of AGNRs.

PDOS of $P_z$ of carbon and of 1s of hydrogen of W9:H(3) (g, h), W9:H(5) (i, j), W10:H(4) (k, l), W10:H(6) (m, n). For instance, “Pz of sp2 C” means the PDOS of $P_z$ of sp$^2$ carbon atoms; “Pz of sp3 C” means the PDOS of $P_z$ of sp$^3$ carbon atoms those bond to the adsorbed H atoms; “1s of edge H” means the PDOS of 1s of H atoms at the edges of AGNRs; and “1s of surface H” means the PDOS of 1s of H atoms adsorbed on AGNRs.
**Figure S2:** Wavefunctions of top valence band (HOMO) and bottom conduction band (LUMO) (at the Γ point) of both edge and surface functionalized AGNRs: H-W-9H, F-W9-H, F-W9-F; H-W10-H, F-W10-H, F-W10-F; W9:H(3), W9:H(5); W10:H(4), and W10:H(6). The isovalue is 0.05. The regions colored by yellow and cyan correspond to the positive and minus part of the wavefunctions, respectively.