Electronic Supplementary Information

How to Achieve Maximum Charge Carrier Loading on Heteroatom-Substituted Graphene Nanoribbon Edges: Density Functional Theory Study

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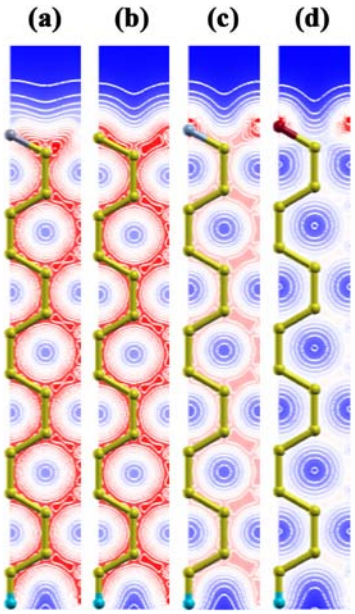

Fig. S1 Total charge density plot for (b) pristine and edge-substituted ZGNRs with (a) boron, (c) nitrogen, and (d) oxygen. The contour interval is set to be 0.005 e/Å^3.

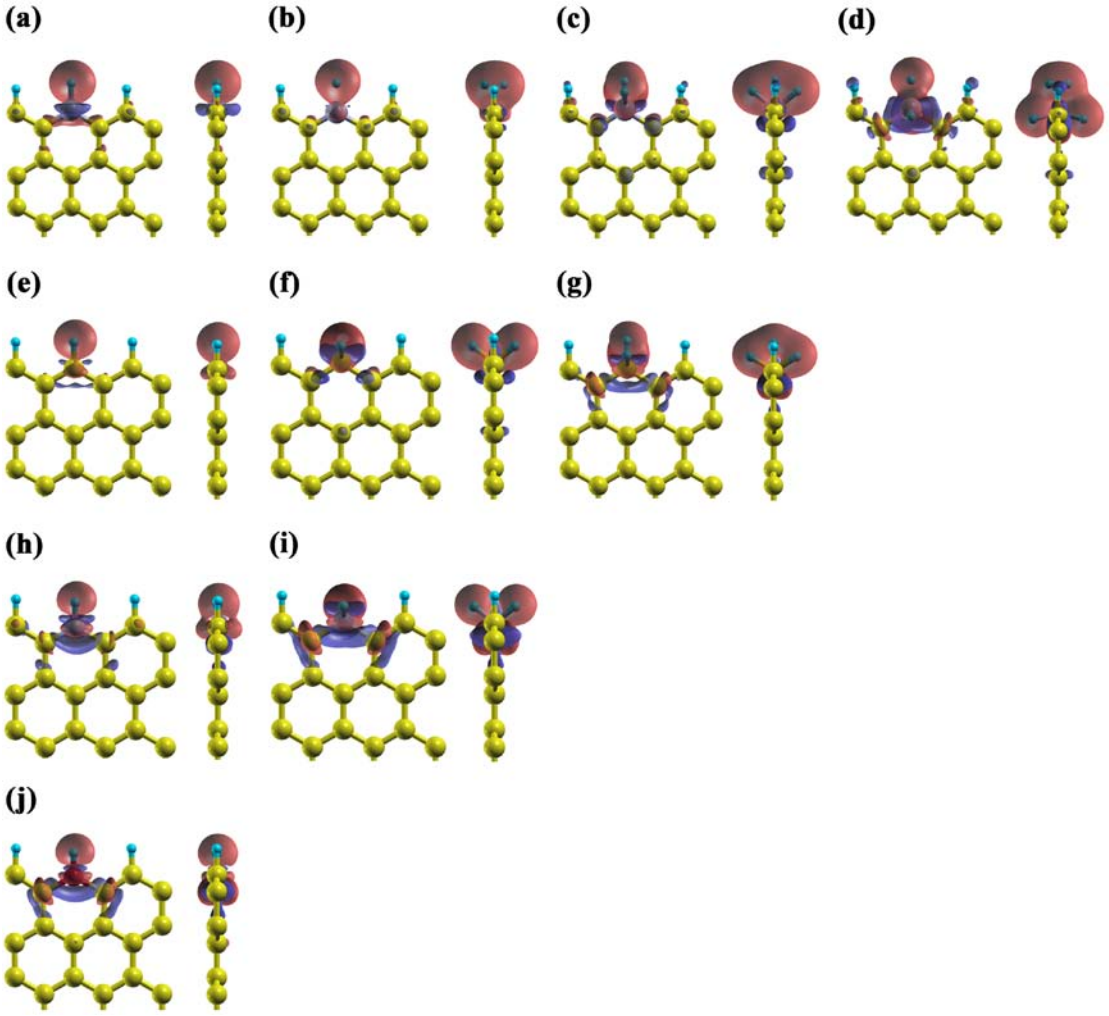

Fig. S2 Front and side views of the charge density difference of protonized ZGNRs with (b) pristine and heteroatom (a) boron, (c) nitrogen and (d) oxygen substituted ribbons. (isovalues for all the isosurfaces are ±0.005 eÅ^{-3}). Only top several atomic layers are shown for better visualization. Red indicates electronic density gain, blue indicates electronic density loss.