Hydrogenation-chain created conduction channels in zigzag graphene nanoribbons

We discover a method of opening the conductive channels of zigzag graphene nanoribbons (ZGNRs) by using hydrogenation chains to separate the nanoribbon into two strips with a ∼ 0.7 Å distance, although the overall hydrogenation on graphene transforms the highly conductive semimetal sheet into an insulator.

The zigzag graphene nanoribbons with edges, terminated by hydrogen atoms, have the strongly localized states (namely edge states) carrying conductive charges. The edge states corresponding to the partly flat band near Fermi energy have large contributions to the density of states. Nakada and coworkers [1] analytically derived the existence of edge states for ZGNRs. In the quantum Hall experiments, the current-carrying localized edge states in the Landau energy gap play an essential role in the Laughlin's gauge invariance argument [2].

We study the role of hydrogenation chains in the process of electronic transport in ZGNRs. In order to enhance the conduction of the graphene nanoribbons, we design modified nanoribbons with one or two carbon chains hydrogenated on opposite faces of the nanoribbon sheet. By elongating the carbon-carbon bonds, the graphane-like hydrogenation chain decreases the conduction ability of the carbon chain and forms a quasi-edge in the central region of the ribbon. On both sides of the hydrogenation carbon chain a new edge-like state appears and enhances the conduction ability of ZGNRs.

Before calculating the transport properties of nanoribbons, we optimize their configurations with B3LYP as exchange-correlation functional, and 6-31g as basis set, convergence on maximum and root-mean-square (RMS) density matrix (10^{-8}), max density matrix (10^{-6}), and energy (10^{-6}) Ry., respectively. The periodic boundary condition (PBC) optimization is done by using 100 k points with the initial structure parameters obtained from a large ZGNR cluster optimization calculation. The hydrogenated carbon atoms are out of the nanoribbon plane due to the bond extension. In Fig. 1, the side view (down pattern) of 7ZGNR2H shows the hydrogenated carbon atoms with distances in Å perpendicular to the ribbon (from top to bottom: 0.43, -0.19, 0.19, and -0.43).

We demonstrate that the hydrogenation chains may have the different effect on conductance of zigzag graphene nanoribbons, although the hydrogenation extends the length of carbon-carbon bond in graphene, and transforms the highly conductive semimetal sheet into an insulator, namely graphane. The hydrogenation chains on ZGNRs open the new edge-like states and enhance the conductive abilities of the ZGNRs by separating the nanoribbon into several narrow strips separated by distance from 0.62 Å(for 7ZGNR2H) to 0.70 (for 7ZGNRH) Å. Furthermore the hydrogenation chains drive the even-

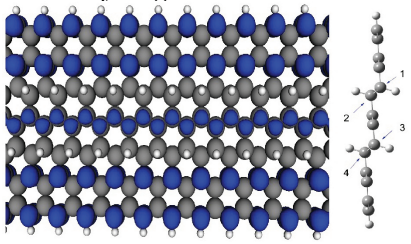

FIG. 1. Configuration and LDOS of 7ZGNR2H. The side view shows the three strips separated by two hydrogenation chains.

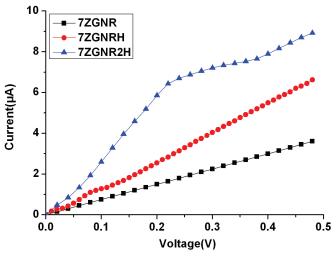

FIG. 2. Current of seven-chain zigzag graphene nanoribbons with/without hydrogenation chains.

row 6ZGNR from a poor conductive state to a metallic one. For 5ZGNRH, we obtain the results (not shown in the paper to avoid duplicate) similar to 7ZGNRH. The fact that each hydrogenation chain creates two conduction channels around itself, which enhances the conductance of ZGNRs, is valid for 5ZGNRH, 7ZGNRH, 7ZGNR2H, and 6ZGNRH. Our numerical calculations demonstrate a novel way for the hydrogenation chains of being used in the nanoelectronics and carbonelectronics engineering.

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Key Words

Edge state, Hydrogenation chain, Nanoribbon

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