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# Contact position and width effect of graphene electrode on the electronic transport properties of dehydrobenzoannulenne molecule under bias

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ABSTRACT

By applying nonequilibrium Green's function formalism in combination with density functional theory, we have investigated the electronic transport properties of dehydrobenzoannulenne molecule attached to different positions of the zigzag graphene nanoribbons (ZGNRs) electrode. The different contact positions are found to drastically turn the transport properties of these systems. The negative differential resistance (NDR) effect can be found when the ZGNRs electrodes are mirror symmetry under the *xz* midplane, and the mechanism of NDR has been explained. Moreover, parity limitation tunneling effect can be found in a certain symmetry two-probe system and it can completely destroy electron tunneling process. The present findings might be useful for the application of ZGNRs-based molecular devices.



## 1. Introduction

Graphene has attracted considerable interest in recent years due to its fantastic properties [1]. Based on graphene, the corresponding quasi-one-dimensional graphene nanoribbons (GNRs) can be obtained by pattering a graphene sheet along one specific direction. Zigzag graphene nanoribbons (ZGNRs) are particularly interesting, and the electronic structure and transport properties of ZGNRs have been intensively theoretically investigated. For instance, Son et al. showed that Armchair graphene nanoribbons (AGNRs) and ZGNRs have a nonzero energy gap, which has been experimentally confirmed by Li et al. and Ritter et al. [2–4]. Li et al. indicated that asymmetric and symmetric ZGNRs show distinctly different transport behaviors due to the symmetry of electron wave functions in these systems [5]. The electronic transport properties of ZGNRs with one or two triangle protrusions at the edge were studied by An et al. [6]. They found that the protrusions can increase or decrease the conductance with different relative position of the protrusions. Most studies as we mentioned have focused on the electronic transport properties of ZGNRs connected to ZGNRs electrodes [5–8]. In this situation, the contact position effects of ZGNRs molecules and ZGNRs electrode have been ignored. Moreover, ZGNRs can form edge states which give rise to flat bands in the electronic band structure and thus to generate a

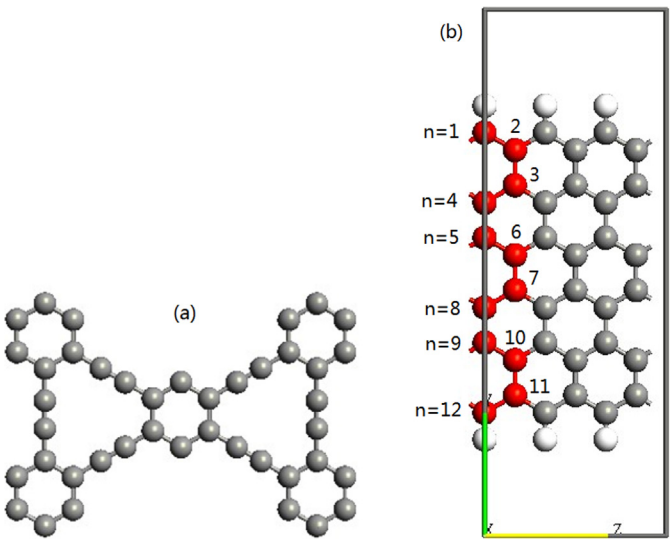


**Fig. 1.** (a) Geometry structure of DBA molecule. (b) Schematic diagram of zigzag graphene nanoribbon electrode. The width is denoted by the carbon number $n$ of dimmer lines (red in the web version). In the paper, $n = 10, 12$ are considered in the calculations.

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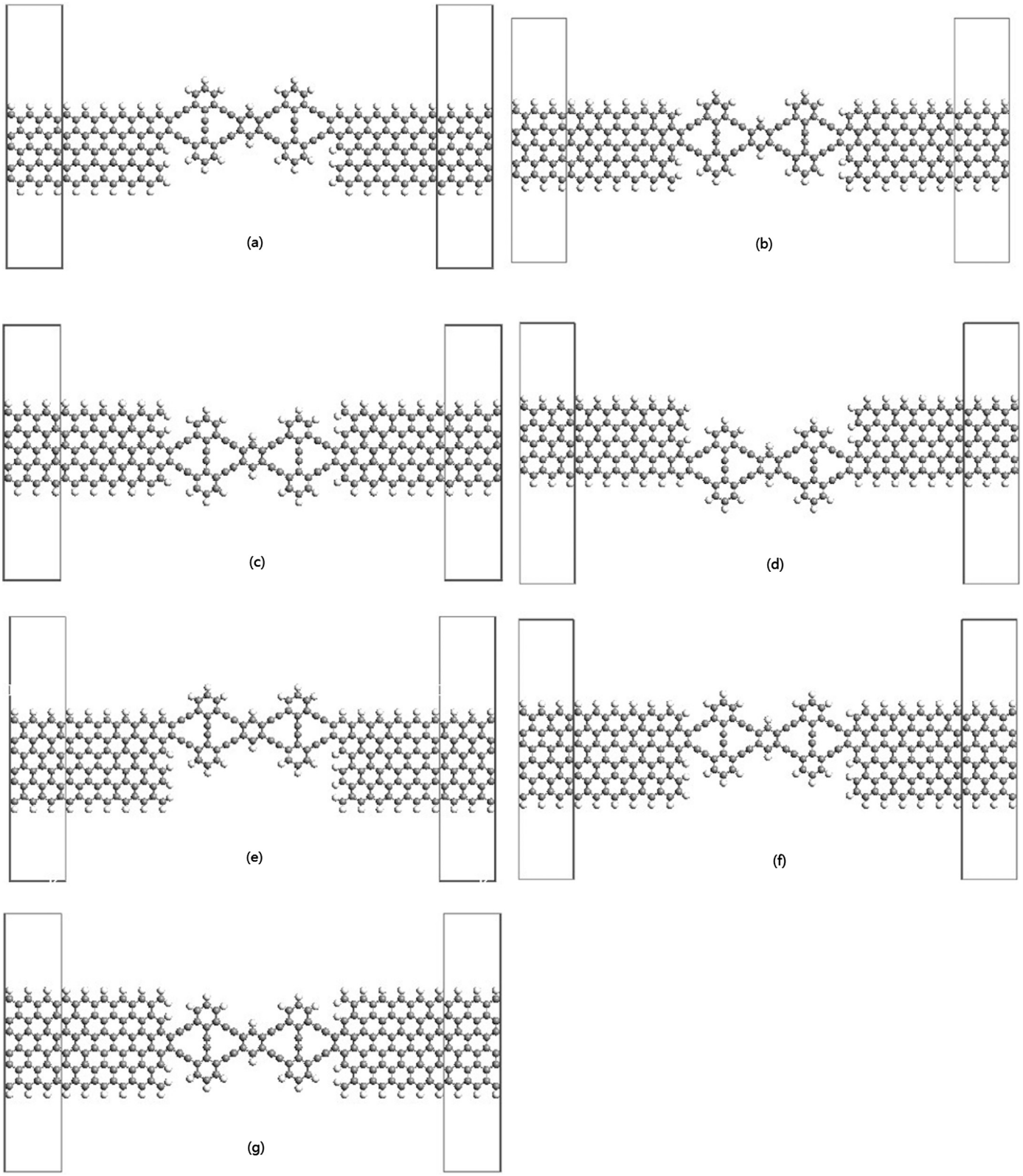


**Fig. 2.** Schematic diagram of the two-probe systems. The rectangle areas indicate the left (L) and right (R) electrodes, between which is the central scattering region. (a) D10EU, (b) D10CU, (c) D10CD, (d) D10ED, (e) D12E, (f) D12CU, (g) D12C.

pronounced peak in the electronic density of state (DOS) at Fermi energy ($E_F$) [2]. This may lead to distinct transport properties when the contact site is edge site or center site. Therefore, it is necessary to systematically study electronic transport properties of molecules connected to ZGNRs electrodes in different contact sites.

In this paper, we use dehydrobenzoannulenne (DBA) for the central molecule as shown in Fig. 1(a), because it possesses good stability, and exhibit little or no sensitivity to heat-, light-, or oxygen-induced decomposition [9,10]. Moreover, DBA is considered as the subunit of graphyne nanoarchitecture [11,12]. Studying for