

## Letter

# Hydrogenation-induced giant rectifying behaviors in silicene and germanene heterojunctions



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## ABSTRACT

By using nonequilibrium Green's function method in combination with density functional theory, the electron transport properties of single atomic chain connected silicene-silicane or germanene-germanane nanoribbon junction are theoretically investigated. Obvious rectifying behaviors with rectification ratios up to  $10^4$  can be obtained by asymmetrically hydrogenating electrodes of the nano junctions. The edge pattern of hydrogenated electrode is shown to play a significant role in determining the rectifying direction of these diodes. Besides, the germanium atoms constructed nano diodes show better rectifying performance than the respective devices constructed by silicon atoms. The rectifying mechanism for these devices is elucidated by analyzing the molecular projected self-consistent Hamiltonian, the transmission spectrum and the band structure of electrodes with applied bias.

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## 1. Introduction

With the miniaturization of electronic devices, molecular electronic units are considered to be a potential substitute beyond the limits of conventional silicon-based semi-conductive devices. Understanding the electronic transport properties of single molecular junctions and further providing molecular devices with high efficiency is an important research field. In recent years, various molecular devices, such as diodes [1,2], switches [3,4], sensors [5,6], negative differential resistance [7,8] and potentiometers [9], have drawn a lot of attention both theoretically and experimentally. Particularly, as an analogue to traditional diode, molecular diode is seen as an essential element to introduce rectifying behavior into the nano integrated circuit. So far, many kinds of molecular diodes have been proposed [10–13]. However, those models are hard to meet the application requirements, which need the diodes have both giant rectification ratio and stable rectifying properties. Therefore, one of the most crucial tasks in molecular diodes study is to find out new models with excellent rectification quality.

Rectification behaviors are caused by asymmetric factors in the diodes. Asymmetric molecular geometry structures, asymmetric electrode materials, asymmetric contact configurations between

molecule and electrodes, and asymmetric environments are frequently-used ways to achieve rectification properties [10,14–18]. In recent years, a great deal of effort has been devoted to pursuing new materials for the development of molecular diodes. Especially the two-dimensional (2D) materials, which have many unique electrical properties, have provided a potential way to design high quality molecular diodes. Previous research have shown that by means of configuration modification, such as doping atoms [13], adsorbing molecules [19], introducing vacancy defects [20], and edge clipping [21], various asymmetric structures could be introduced into molecular devices, so that one-atom-thick rectification models were proposed. Recently, a novel modifying technique for 2D materials has drawn extensive interest. Experiments have shown that a single atomic sheet of graphene, silicene and germanene can be completely hydrogenated, and transform into graphane, silicane and germanane, respectively [22–24]. After reacting with atomic hydrogen, the carbon (silicon or germanium) atoms in pristine sheet will change from sp<sup>2</sup>-hybridization (or mixed sp<sup>2</sup>-sp<sup>3</sup>-hybridization) into sp<sup>3</sup>-hybridization, inducing completely different electronic properties in 2D materials [25,26]. Therefore, molecular diode can be created by hydrogenating one of the electrodes in a nano junction. Importantly, an advantage of these devices is that the rectifying direction is tunable due to the reversible hydrogenation property [23,27]. In addition, electrical properties of 2D-material-based nanoribbons are extremely sensitive to their edge geometries. For instance, after saturating both edges of silicene nanoribbons (SiNRs) with hydrogen atoms,

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zigzag edged SiNRs (zSiNRs) are shown to be zero band gap materials, whereas armchair edged SiNRs (aSiNRs) are semiconductors with obvious energy gaps [28]. Thus, if zSiNRs and aSiNRs are respectively employed in a diode, different rectifying behaviors might be witnessed.

All in all, although the hydrogenated effects in one-atom-thick 2D material have been studied both experimentally and theoretically [22–27], their applications in molecular diodes have not been studied yet. Motivated by this, we design a nano-scale junction constructed by a silicon atomic chain sandwiched between a SiNR and a hydrogenated SiNR. In order to reveal the edge effect of nanoribbon in rectification, both zigzag edged and armchair edged ribbons are studied. Besides, germanium-based devices are also prepared to compare with silicon-based ones in this work. Based on the first principles calculation, the electronic transport properties and rectification effects of these nano diodes are investigated. We present an interesting result that giant rectifying behaviors can be obtained by hydrogenating one of the electrodes, and the edge patterns of hydrogenated nanoribbons play an essential role in regulating the rectifying direction of these diodes. Moreover, the band structures and transmission spectra are analyzed to give insight into the physical mechanisms of rectifying behaviors in these devices.

## 2. Computational details

In this work, all the geometric structure relaxation and electronic structure optimization are carried out based on the first principles calculations, as implemented in the SIESTA package [29]. The local density approximation (LDA) [30] is used for the exchange-correlation functional, which have been proved to be a suitable choice in calculating materials based on elements of group IV [31]. The basis set is described by the numerical atomic orbitals, and the Troullier-Martin-type norm-conserving pseudopotentials are employed for modeling the core electrons [32]. In order to generate the pseudoatomic orbitals' cutoff radii systematically, the energy shift parameter of 100 meV is adopted in the calculation. The atoms in this work are represented by a single- $\zeta$  plus single polarization (SZP) basis set, and the mesh cutoff sample for the real space grid is set as 300 Ry to balance the computation time and the calculation accuracy. Based on the Monkhorst-Pack scheme, a  $1 \times 1 \times 100$   $k$ -point grid is used for the Brillouin zone. The geometries of these devices are fully relaxed until the force is less than the tolerance limit  $0.02 \text{ eV \AA}^{-1}$ , and the density matrix is self-consistent iterated with a convergent criterion of  $10^{-4}$ .

The calculation of electronic transport property is carried out by using the TranSIESTA module [33], which combines the density functional theory (DFT) with the nonequilibrium Green's function (NEGF) technique [34,35]. The current through the central scattering region is calculated by the Landauer-Büttiker formula [36], which is written as

$$I = \frac{2e}{h} \int T(E, V) [f(E - \mu_L) - f(E - \mu_R)] dE, \quad (1)$$

where  $e$  is the electron charge,  $h$  is the Planck constant,  $\mu_{L(R)}$  is the electrochemical potential of the left (right) electrode and  $f$  is the Fermi-Dirac distribution function.  $T(E, V)$  is the electronic transmission coefficient under bias voltage  $V$ , which is defined as

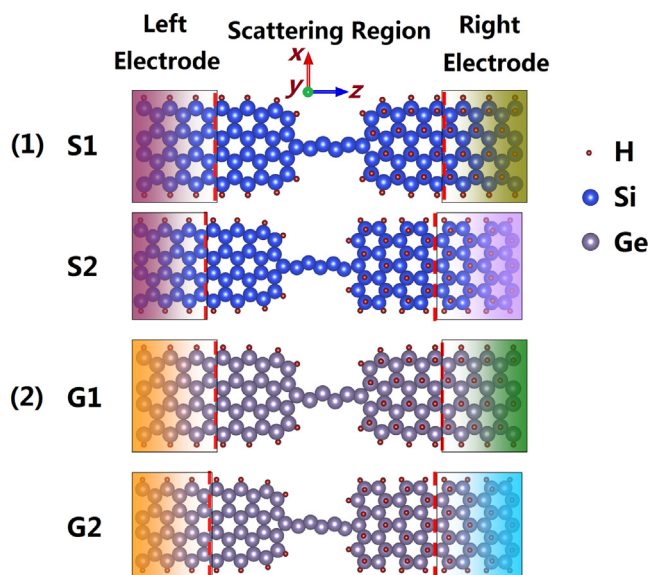
$$T(E, V) = \text{Tr}[\Gamma_L G_M^r \Gamma_R G_M^a], \quad (2)$$

where  $\Gamma_{L(R)} = i[\sum_{L(R)}^r - \sum_{L(R)}^a]$  is the coupling matrix between the left (right) electrode and the central scattering region,  $G_M^{r(a)}$  is the retarded (advanced) Green's function of the central scattering region.

## 3. Results and discussion

The proposed nano diodes are illustrated in Fig. 1, in which S series (S1 and S2) and G series (G1 and G2) are based on silicon and germanium, respectively. In these computational models, two semi-infinite nanoribbon are connected by a six atoms formed single atomic chain. In order to investigate the rectifying effect in these molecular diodes, the asymmetric configuration is adopted, i.e., one of the semi-infinite nanoribbon in a junction is hydrogenated. When silicene and germanene are hydrogenated into silicane and germanane, the hybridization of silicon and germanium atoms is changed from mixed  $sp^2$ - $sp^3$ -hybridization to  $sp^3$ -hybridization, making the buckled formation more obvious [25,26]. In detail, some typical geometric parameters of the optimized nano junctions are presented in Table 1. From the height differences between adjacent atoms, one can see that both pristine SiNR and GeNR are low-buckled, which is corresponding with previous researches [37–39]. When they are saturated by hydrogen atoms, the height differences enlarge more than  $0.15 \text{ \AA}$ , namely, the buckled structure in nanoribbon is much more obvious under the effect of hydrogenation.

As illustrated in Fig. 1a, device S1 is constructed by a six-silicon-atomic chain, which is sandwiched between a zigzag edged silicene nanoribbon (zSiNR) and a zigzag edged silicane nanoribbon (zSiHNR). And junction S2 is a device in which a zSiNR and an armchair edged silicane nanoribbon (aSiHNR) are anchored together by a six-atomic chain as junction S1. From previous researches, we know that carbon-based single atomic chains can be alternating single-triple bonded polyynes or continuous double bonded cumulene, which is dependent on the even or odd number of atoms [21,40]. Being similar with carbon materials, silicon-based atomic chains also have various bonding ways. Since the aSiHNR has a top atom to connect with the central chain, bonds of silicon-based atomic chains in device S1 and S2 are distinct from each other. Then, different conducting properties can be predicted in S1 and S2. In Fig. 1b, devices G1 and G2 are constructed by



**Fig. 1.** Schematic of nano junctions with different electrodes: crimson, pristine zSiNR; claybank, hydrogenated zSiNR; purple, hydrogenated aSiNR; orange, pristine zGeNR; green, hydrogenated zGeNR; blue, hydrogenated aGeNR. (1) Molecular junctions based on silicon atoms, denoted as S1 and S2. (2) Molecular junctions based on germanium atoms, denoted as G1 and G2. The region between the two vertical dashed lines is the scattering region. The center six-atomic chain is the molecular part. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

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