



Adsorption and Diffusion Energies Calculation of Sodium Ion Battery using GeTe Anode : A Density Functional Theory Study

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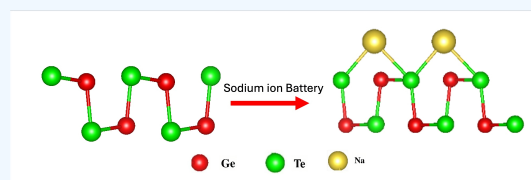
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ABSTRACT

Sodium batteries are the most potential candidates for future and green energies storage systems. However, there are problems with structural instability in the electrodes, which affect battery performance. Therefore, this study investigated the adsorption and diffusion mechanisms at the anode using a phase puckered Germanium Telluride (GeTe) monolayer structure. Density functional theory (DFT) calculations show that the Na-adsorbed hollow Te-Te structure is the most stable adsorption configuration (-1.25 eV). In the diffusion scheme, Na atoms move through the hollow Te-Te (initial state) followed by the hollow Ge-Ge (transition state), then to the hollow Te-Te (final state). The diffusion mechanism that occurs has lowest energy of 0.09×10^{-4} eV. These results suggest that the phase puckered GeTe monolayer has the potential as a high-performance sodium battery anode.

Keywords: Sodium Battery, Germanium Telluride (GeTe), DFT, adsorption, Diffusion, Puckered



1. INTRODUCTION

Advances in portable electronic devices, smart grids, and electric vehicles have led to increased efficiency in energy storage systems [1, 2]. The most dominant green energy storage system used today is rechargeable batteries [3]. There are several types of rechargeable batteries, such as lithium, sodium, potassium, and aluminum [4, 5, 6, 7]. Based on these battery types, lithium batteries show good performance compared to other battery types [8, 9, 10]. Lithium batteries have advantages such as high energy density and good power density [11, 12]. However, the availability of lithium is limited, and the operational cost is expensive, so an alternative to lithium batteries is needed.

Sodium batteries are the most potential candidate as a replacement for lithium batteries [13, 14, 15, 16, 17, 18, 19]. This is based on its low price and abundant availability in nature [17]. In addition, sodium batteries have disadvantages including a larger atomic radius than lithium, low energy density, poor cycle life, and poor volume expansion during the charging/discharging process [20, 21]. So, to overcome these weaknesses, further development is needed on the electrode component [22]. Electrode components consist of cathode, anode and SEI [23, 24]. Based on the three components, the anode has an important role in improving battery performance [25]. In this study, germanium telluride (GeTe) is considered as a promising anode for sodium batteries [2, 26, 27, 28]. GeTe has been reported as an anode in batteries and other devices (such as electronic devices, thermoelectric, electrodes) [2, 29, 30, 31]. However, the issue of sodium atom adsorption mechanism on GeTe anode is still unclear.

Investigating the structure and phase of GeTe on sodium

battery anodes can help to understand the mechanism that occurs. The structure used is monolayer because it has advantages such as high theoretical capacity, fast sodiation kinetics, able to increase stability, can reduce structural instability and electrolyte decomposition [9, 11, 12, 15, 27, 32, 33]. The puckered phase is an option in designing anodes because it has good ion diffusion [2], shows high theoretical capacity and good cycle stability [34, 35]. Thus, the phase puckered monolayer structure has potential as a high-performance anode. Based on its potential, an understanding of adsorption and diffusion is needed. Therefore, this study varies the placement of Na atoms (such as top Ge, top Te, hollow Ge-Ge, hollow Te-Te, bridge upper, bridge lower and middle) to determine the adsorption and diffusion that occurs in monolayer phase puckered GeTe using density functional theory (DFT).

2. METHODS

In this study, the density functional theory was performed using Quantum ESPRESSO [36, 37], which aims to determine the adsorption and diffusion energy in puckered GeTe. The calculation parameters we set 50 Ry and 500 Ry for charge and wavefunction cutoff, respectively. We further set the convergence threshold by 10^{-8} Ry. In order to perform the calculation more accurately, we used the PBE3 functional with ONCV pseudopotential. We used a vacuum slab 15 Å to remove the interaction of the slab repetitions. The k-point mesh variation ($6 \times 6 \times 1$), ($8 \times 8 \times 1$), ($10 \times 10 \times 1$) and (2×2) unit cells.

To calculate the adsorption energy (E_{ads}) the following

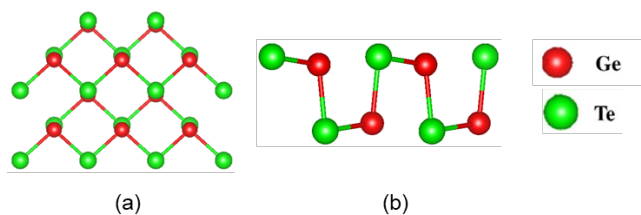


Figure 1. Clean surface phase puckered GeTe: (a) Top view, (b) Side view

equation was used,

$$E_{ads} = (E_{Total} - (E_{Surface} + E_{Isolated})) \quad (1)$$

where the total energy (E_{total}) shows the energy of Na atoms adsorbed on the puckered GeTe monolayer, the surface energy ($E_{surface}$) shows the energy of the clean surface structure. Whereas the isolated energy ($E_{isolated}$) represents the energy of Na atoms during the vacuum state in the system. The Diffusion energies (E_{diff}) were calculated by compared between the most stable E_{ads} with the nearest neighbor E_{ads} .

To further understand the adsorption properties, we investigated the charge density of various sites of GeTe's monolayer phase puckered structure using the equation of

$$\Delta\rho(r) = \rho_{total}(r) - \rho_{surface}(r) - \rho_{molecule}(r) \quad (2)$$

where ρ_{total} is the charge density of Na atoms adsorbed on puckered GeTe, $\rho_{surface}$ is the charge density of clean surface puckered GeTe and $\rho_{molecule}$ is the charge density of isolated Na atoms.

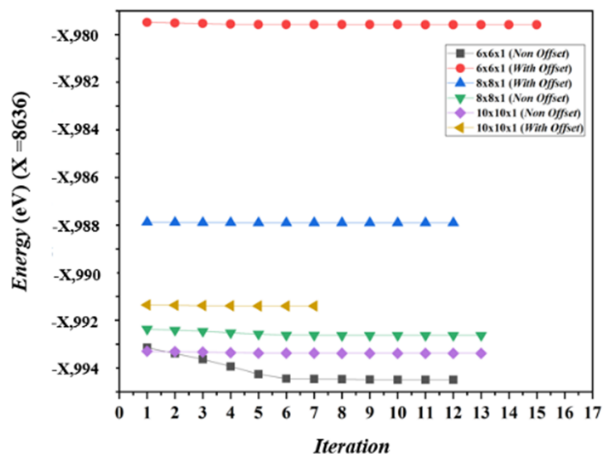


Figure 2. Calculated total energy of clean GeTe with k-point mesh and grid variations

3. RESULTS AND DISCUSSION

3.1 Clean Surface Phase Puckered GeTe

Phase puckered GeTe is a two-dimensional crystal structure. Puckered GeTe is formed due to a phase transition that is displacive in the GeTe honeycomb crystal. The displacive nature is the movement of atoms in the crystal lattice that forms the puckered phase. We investigated the clean surface (see Figure 1) with variation of k-point mesh and grid (non offset and with offset). The results show that k-point mesh with non offset grid has significant results in achieving equilibrium, and the k-point used is $6 \times 6 \times 1$ (Figure 2).

3.2 Na Adsorption on Monolayer Phase Puckered GeTe

To determine the adsorption properties of Na atoms on the monolayer phase puckered GeTe structure, we consider various adsorption site, namely bridge, hollow, top and middle. Those sites are similar with previous research by putra et al. [38]. At the top site, Na atoms are placed above Ge and Te atoms. Middle site, Na atoms are located in the middle of the structure. The placement of Na atoms at the bridge site is at the top and bottom of the structure, while at the hollow site Na atoms are in the Te-Te and Ge-Ge hollows. We found that the Te-Te hollow site is the most stable adsorption site, as seen in Figure 3. The calculated adsorption energies of the Te-Te hollow adsorption site are -1.25 eV. The minus adsorption energies represent a stronger interaction between Na atoms and puckered GeTe, and a negative value indicates an exothermic reaction. The distance between the surface (Te atom) and Na atom 3.198 until 3.358 Å. While the distance to the Ge atoms is around 0.2 Å larger than that Na-Te atoms distances. These indicated that the Na-Te or Na-Ge atom introduce similar interaction with the adsorbed atoms. These calculated results also in good agreement with the previous results, which mention the hollow site give the stronger adsorption energies [38].

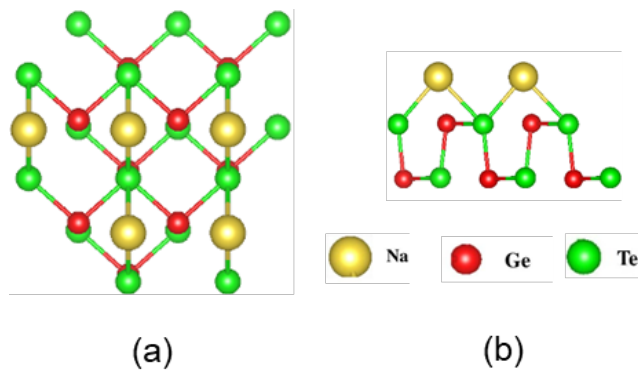


Figure 3. Most stable adsorption site of Na atom on GeTe puckered phase from (a) top and (b) side views. The yellow, red, and green spheres represent the sodium, germanium, and tellurium atoms respectively.

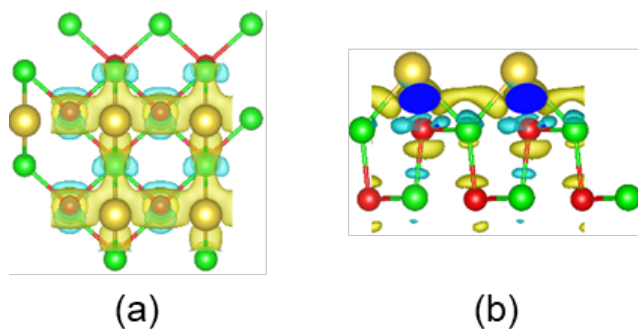


Figure 4. The calculated charge density difference of the most stable adsorption site of Na atom on GeTe puckered phase from (a) top and (b) side views. The cyan and yellow color represent the loss of electrons and gain of electrons on the atom, respectively.

Our calculated results further indicated that the Na atoms adsorbed on monolayer phase puckered GeTe show a change

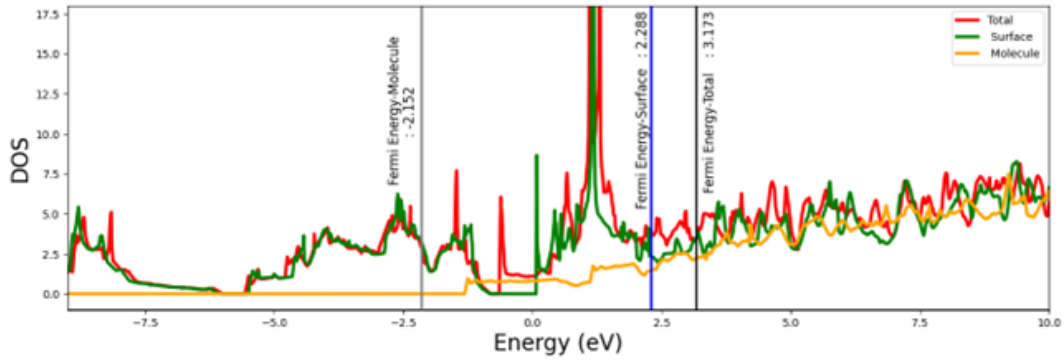


Figure 5. The calculated Density of States (DOS) of adsorbed Na over GeTe puckered surface. The red, green, and yellow represents the calculated DoS of total, GeTe surface, and Na molecules, respectively.

in bond length. Na-Te and Ge-Te are bonds that experience changes in bond length after optimization results. This change can explain the interaction between atoms related to the potential energy surface (PES) [39]. According to the PES concept, the difference in bond length is caused by repulsion [40]. The shorter bond length represents the repulsive force between atoms is stronger than the force of attraction, while the longer bond length applies the opposite.

The condition of Na atoms after optimization tends to interact with Te atoms. This is influenced by the atoms vibrating with each other. In our case, the size of the atomic radii (Na > Te > Ge) affects the vibrating atoms, the formation of bent bonds and the bond angles in Te-Na (see figure after optimization). In addition, we verified the bond length optimization calculation results with experimental results and reference DFT calculations.

In order to explain the interaction between Na and the surface, we investigated the charge density difference. Figure 4 shows the charge density of the investigated sites. The cyan color represents the loss of electrons, and the yellow color represents the gain of electrons on the atom. The largest charge difference is located around the Na atom, while the adjacent atoms (Ge and Te) show excess charge. Thus, this structure has ionic characteristics.

We also calculated the density of state (DOS) of various sites shown in Figure 5. After the clean surface structure is adsorbed by Na atoms, there is an increase in energy around the fermi area. The increase represents metallic properties that are beneficial in the conduction of electricity in the SIB anode. It can be observed that there is overlap between ρ total, ρ surface and ρ molecule which indicates covalent hybridization. The results of this investigation suggest that monolayer phase puckered GeTe is dominated by covalent bonds and ionic interactions.

3.3 Mechanism of Diffusion

The diffusion energy values in Table 1 show that Na atoms can move from the most stable adsorption site as the initial state (hollow Te-Te) to the nearest neighbor site and to the final state (hollow Te-Te) through transition states such as top Te, hollow Ge-Ge, bridge Te-Te, bridge upper, top Ge, middle, bridge lower. Table 3 also shows that the diffusion scheme of Na atoms through hollow Ge-Ge gives the smallest diffusion energy (0.09×10^{-4} eV). In addition, diffusion at bridge Te-Te (16.3×10^{-4} eV), top Ge (16.4×10^{-4} eV), bridge upper (16.3×10^{-4} eV) sites shows the next most probable diffusion scheme. Based on the possible diffusion schemes

occurring in Na-adsorbed puckered GeTe, the 3rd diffusion scheme (Figure 6(c)) becomes the most probable scheme due to the smallest diffusion energy. The diffusion mechanism in the 3rd scheme shows Na atoms moving through hollow Te-Te (initial state) and then through hollow Ge-Ge (transition state) to reach the final state. (hollow Te-Te).

Table 1. The most stable diffusion energy in the puckered phase of GeTe adsorbed with Na.

Diffusion schemes	Diffusion Energies (eV)
Hollow Te-Te to Bridge Te-Te	16.3×10^{-4}
Hollow Te-Te to Bridge upper	16.3×10^{-4}
Hollow Te-Te to Bridge lower	239.5×10^{-4}
Hollow Te-Te to Top Ge	16.4×10^{-4}
Hollow Te-Te to Hollow Ge-Ge	0.09×10^{-4}
Hollow Te-Te to Middle	238.7×10^{-4}
Hollow Te-Te to Top Te	0.2×10^{-4}

In the diffusion process, temperature is one of the parameters in influencing the diffusion mechanism so that it will have an impact on battery performance. Based on the Boltzman equation or thermal energy equation as follows.

$$E_t = k_B \times T \tag{3}$$

Where E_t is the thermal energy, k_B is Boltzman's constant, and T is the temperature. At 300 K the required thermal energy is 1.70112×10^{-2} eV/K. While in the 3rd scheme diffusion process with a diffusion energy of about 0.09×10^{-4} eV. This shows that Na atoms have diffused at 300 K. In addition, this study also considers the diffusion energy of other DFT-based materials. The energy comparison results in Table 1 show that monolayer phase puckered GeTe can be a high-performance sodium battery anode material.

4. CONCLUSION

We have successfully calculated the adsorption and diffusion energies of Na atom adsorption on GeTe puckered phase surface. We found that the Na-adsorbed hollow Te-Te structure is the most stable adsorption configuration (-1.25 eV). The diffusion mechanism that occurs has the lowest energy of 0.09×10^{-4} eV. These results suggest that the phase puckered GeTe monolayer has the potential as a high-performance sodium battery anode. Further investigations are needed to confirm the ability the GeTe as anode in sodium batteries.

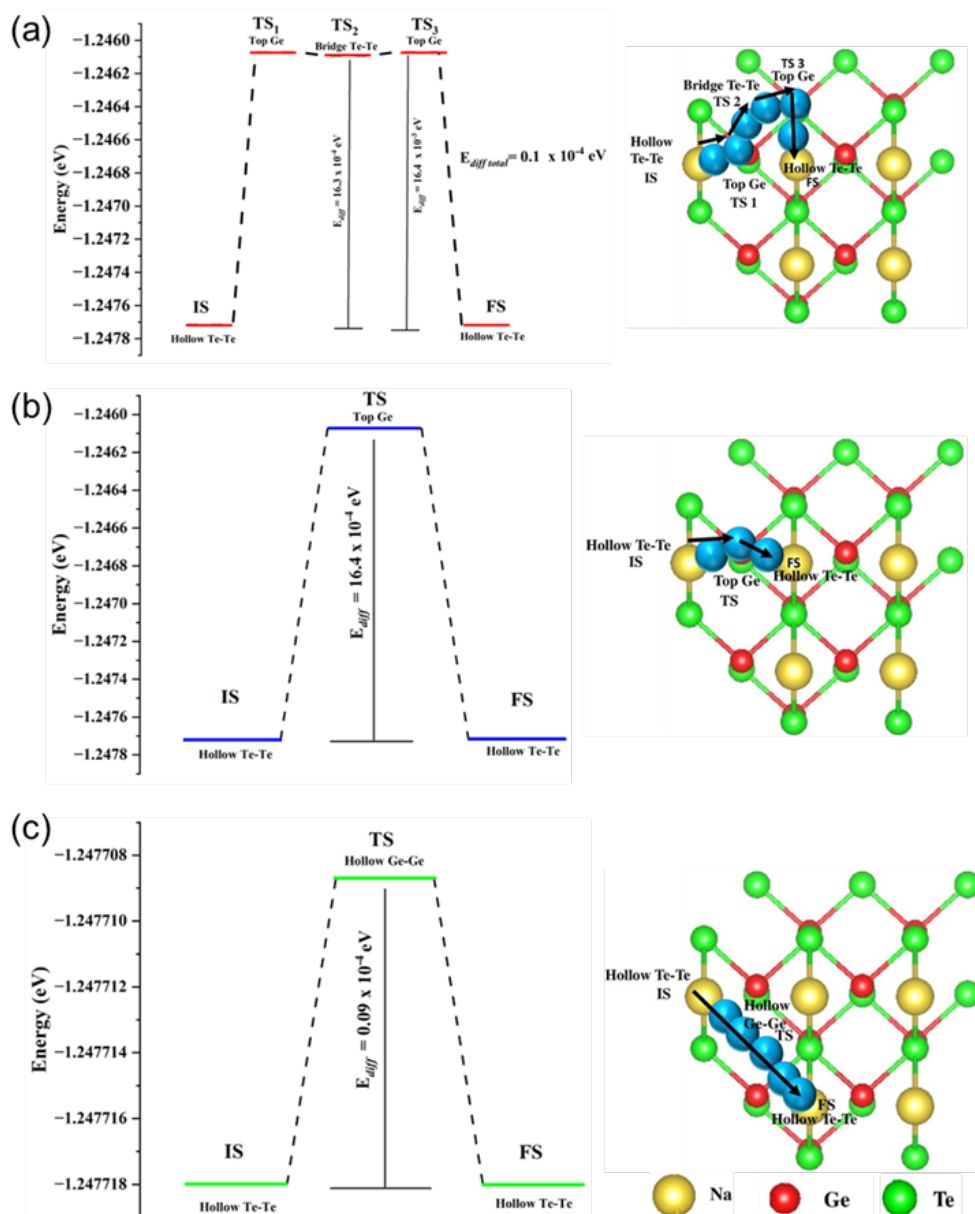


Figure 6. Diffusion schemes of Na-adsorbed puckered GeTe: (a) 1st diffusion scheme, (b) 2nd diffusion scheme, (c) 3rd diffusion scheme. IS (initial state), TS (transition state), FS (final state)

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