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Ca and K decorated germanene as hydrogen storage: An ab initio study

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ABSTRACT

The hydrogen storage capacity and performance of Ca and K decorated germanene were studied using density functional theory calculation. The Ca and K adatoms were found to be sufficiently bonded to the germanene without clustering at the hollow site. Further investigation has shown an ionic bonding is apparent based on the charge density difference and Bader charge analysis. Upon adsorption of H₂ on the decorated germanene, it was found that the Ca and K decorated systems could adsorb 8 and 9 H₂ molecules, respectively. The adsorption energies of H₂ molecules were within the Van der Waals energy (400–435 meV), suggesting weak physisorption. The charge density profile revealed that the electron of H₂ moved toward the adatom decoration without leaving the local region of H₂. This suggests that a dipole-dipole interaction was apparent and consistent with the energy range found. Finally, the gravimetric density obtained from the adsorption of H₂ on the decorated germanene shows that this material is a potential for H₂ storage media.

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Introduction

With the impending depletion of fossil fuel reserves, significant effort has been expended in the development and implementation of technologies for sustainable alternative energy resources [1–4]. One of the potential alternatives is utilizing hydrogen as an energy source. Hydrogen is abundant in nature and when made into an energy carrier, it can be considered as a clean synthetic fuel. Hydrogen is being considered as an energy carrier due to its high gravimetric energy density, safety manageability, and environmentally benign nature of combustion [5–7]. Although the use of

hydrogen might seem ideal, there is still a lot of room for development in the production and storage aspects [8–11]. Between the two facets of hydrogen-based energy, the storage aspect poses the most significant impact in realizing the hydrogen industry. To compare, hydrocarbon and hydrogen can be stored at 1000 kg m⁻³ and 71 kg m⁻³ [7], respectively. Storage technologies such as pressurized gas tank and cryogenic liquid storage are already in development. However, the use of such technologies for mobile application poses safety and weight concerns [12–15].

An alternative storage can be constructed through material-based approach where the material stores the hydrogen by weak interactions. Chemisorption and

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physisorption are means that can be utilized for the attraction. However, chemisorption due its strong bonding poses a challenge on the extraction energy requirement of the stored hydrogen, which leaves physisorption to be of better approach [16]. The main advantage of physisorption mechanism is that it produces materials with lightweight property, and quick H_2 recharge and extraction rate. On the other hand, physisorption method has the lowest hydrogen yield among the available storage methods [16].

In the material-based approach, investigations are typically done through density functional theory (DFT) simulations and experiments on bulk surfaces and nanostructures such as graphene, nanoribbon, nanoring, and fullerene. Graphene and single-walled carbon nanotubes, two nanostructures commonly known with the largest surface areas, yield hydrogen storage capacity below the standard set by the department of energy [16,17]. In response to this challenge, studies have been conducted in exploring possible functionalization of the materials to increase the hydrogen storage capacity [18–24]. It was shown that decoration and doping could indeed increase the hydrogen storage capacity of the material [25–30]. In decorated graphene studies, the metal decoration was observed to likely form a cluster due to lower binding energy as compared to its cohesive energy [31,32]. Upon further investigation, this cluster formation was found to decrease the hydrogen storage capacity by inhibiting

hydrogen approach and attraction. Thus, it was recommended that the decorations be in isolated states [33]. Since graphene cannot hold decorations in isolated states, silicene (a graphene allotrope made of Si) was preferred since it was found to keep the decorations bound in isolated states [31,34]. Furthermore, Na, Ca, Mg, and K decorated silicene was said to exceed the hydrogen storage capacity goal of 5.5 wt% [35].

Germanene, a Ge allotrope akin to silicene, has been recently synthesized on gold substrate [36]. Germanene has a similar structure with silicene but with a larger interatomic distance and buckling height [37]. Studies have been conducted to investigate the structural, electronic and hydrogen interaction aspects of germanene [37–41]. However, metal decorations and their capability in storing hydrogen are not yet extensively elucidated. Due to the high uptake potential of materials decorated with K and Ca [35,42,43], these two were chosen as the decoration for the germanene substrate. In this study, the various properties such as the structure, electronic nature, binding mechanism, and hydrogen storage capacity of the K and Ca decorated material were examined.

Methodology

The study utilized spin-polarized density functional theory calculations through the Vienna Ab initio simulation package

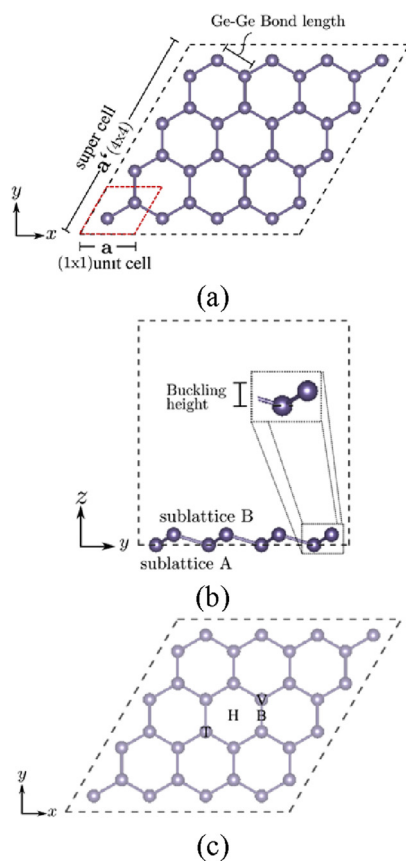


Fig. 1 – Geometry visualization of germanene from the top (a) and side (b) view. The binding sites for the Ca and K are shown in (c).

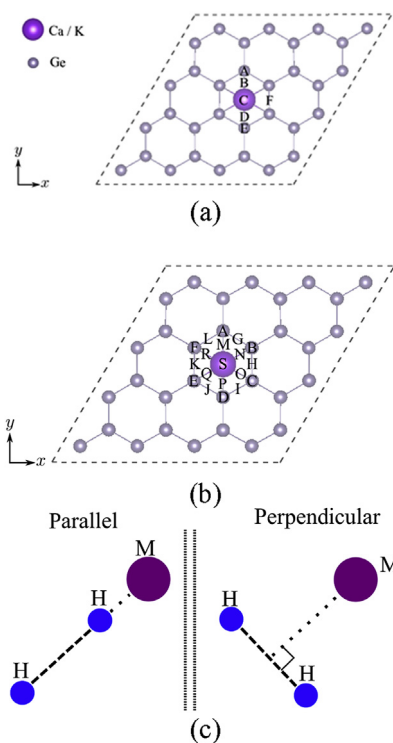


Fig. 2 – The adsorption sites for the 1st H_2 are labeled from A-F in (a). From the 2nd H_2 onwards, there are more adsorption sites to be considered due to the removal of symmetry as an effect of the 1st H_2 . The adsorption sites for the 2nd H_2 onwards is described by sites A-S of in (b). Two initial orientations were considered for approach of hydrogen, the parallel (left) and perpendicular (right) with respect to the Metal (M) decoration.

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