THE EVOLUTION IN CHARACTERISTICS OF GERMANENE UPON HYDROGENATION

Hanh T.T. Tran, Hoang H. Mai, Hang T.T. Nguyen, Hoang V. Vo

The Applied Science Faculty, Ho Chi Minh City University of Technology, VNU-HCM, Ho Chi Minh City, Viet Nam

1. INTRODUCTION

- Germanene have potential of hydrogen-storage material.
- Germanene has been evaluated for capture of gas such as NO, CO and CO2 but not been tested in hydrogen storage.
- Fixed germanene to adsorbed full hydro on two top position (low and high buckling).

2. CALCULATION METHODS

We using SIESTA software to perform DFT simulation with following parameters:

- GGA-PBE.
- The Monkhorst-Pack special k point of 5x5x1 meshes.
- The energy mesh-cutoff for plane-wave basis set is 300 Ry.
- For band structure and phonon calculation, k-point of 21x21x1 meshes and energy mesh-cutoff 500 Ry

3. RESULTS AND DISCUSSIONS

3.1 The adsorption energies and crystal structure.

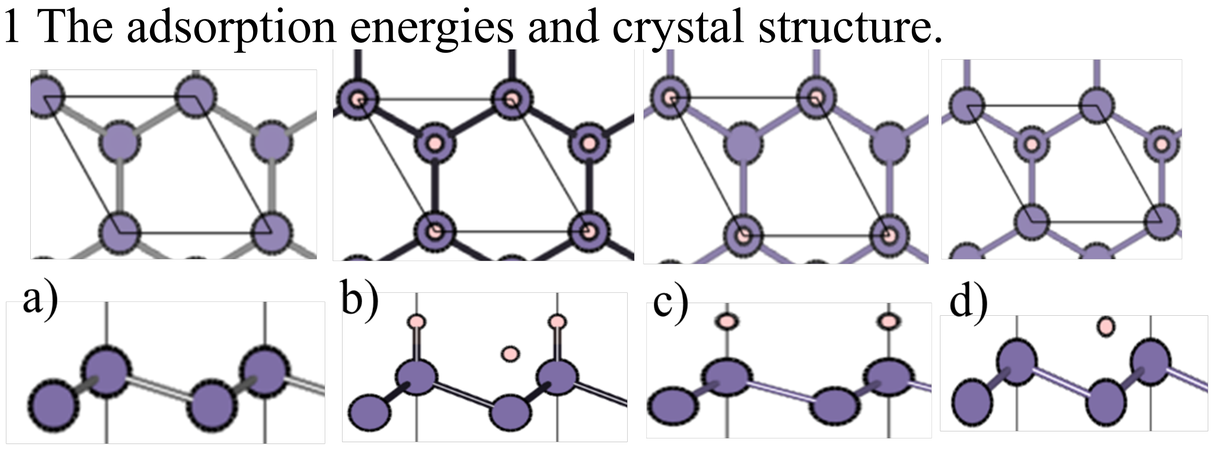

Figure 1. The top and side view of structure of optimized germanene and hydronated germanene: a) germanene, b) full hydro germanene, c) T1 hydro germanene, d) T2 hydro germanene.

- The lattice constant does not change throughout the hydro adsorption. This is a difference from other research.
- The bonding lengths, bond angles of germanene and its derivatives was presented.

Table 1. The calculated bonding lengths (d), lattice constant (a) and bond angles ()of germanene and its derivatives

	Germanene	FH	T1	T2
d(Ge-Ge) Å	2.46469	2.57014	2.49786	2.52807
d(Ge-H) Å		1.58736 (with high buckling Top1), 1.69198 (with low buckling Top2)	1.60470	1.72598
∠(Ge-Ge-Ge)°	111.7158	105.0633	109.5027	107.5891
∠(Ge-H-Ge)°		70.8356	74.0259	110.0048
ΔZ Å	0.72556	1.02829	0.83129	0.91806
a Å	24.478880448	24.478880448	24.478880448	24.478880448

❖ The adsorption energies of three models hydro-adsorpted were calculated using:

$$E_{ads} = E_{germanene-n_H} - E_{germanene} - n_H E_H$$

E_{ads}: the adsorption energy
$E_{germanene\text{-}nH}$: the total energy of the combined system Ge and hydro
$E_{germanene}$: the total energy of the Ge
n_H: the quantity of hydro adsorpted on Ge
E_H: the total energy of hydro

Table 2. The adsorption energy of three models adsorpted hydro.

		FH	T1	T2
$E_{germanene-n_H}$	(eV)	-8789.726504	-8217.758524	-8207.310806
$E_{germanene}$	(eV)	-7676.656674	-7676.656674	-7676.656674
E_H	(eV)	-12.093984	-12.093984	-12.093984
n_H		72	36	36
E_{ads}	(eV)	-242.302982	-105.718426	-95.270708
E_{ads} / n_H	(eV)	-3.365319194	-2.936622944	-2.646408556

3.2 The band structure and phonon spectra of three models adsorpted hydro.

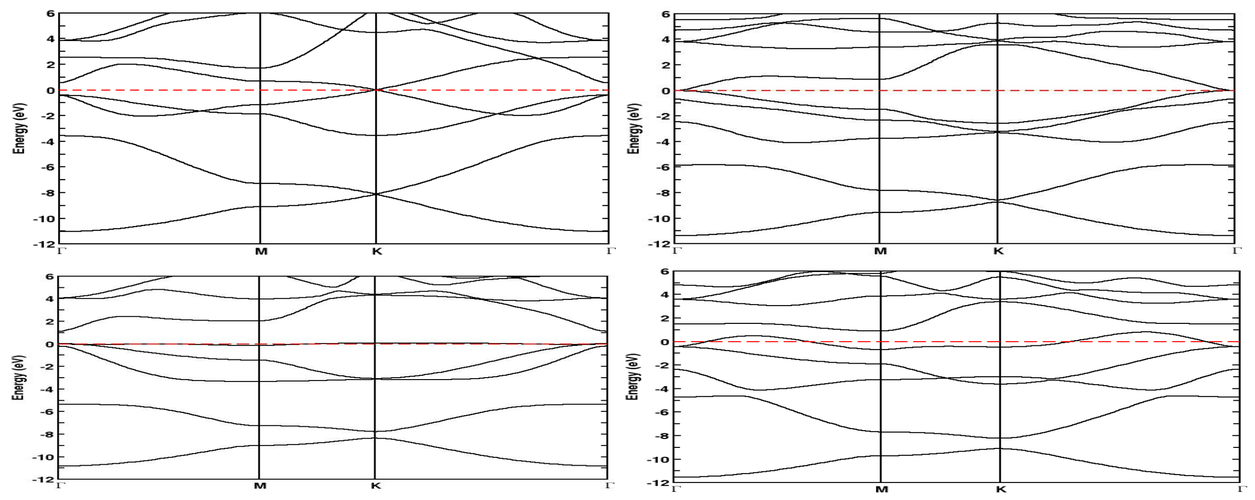

Figure 2. Band structure of three models adsorpted hydro.

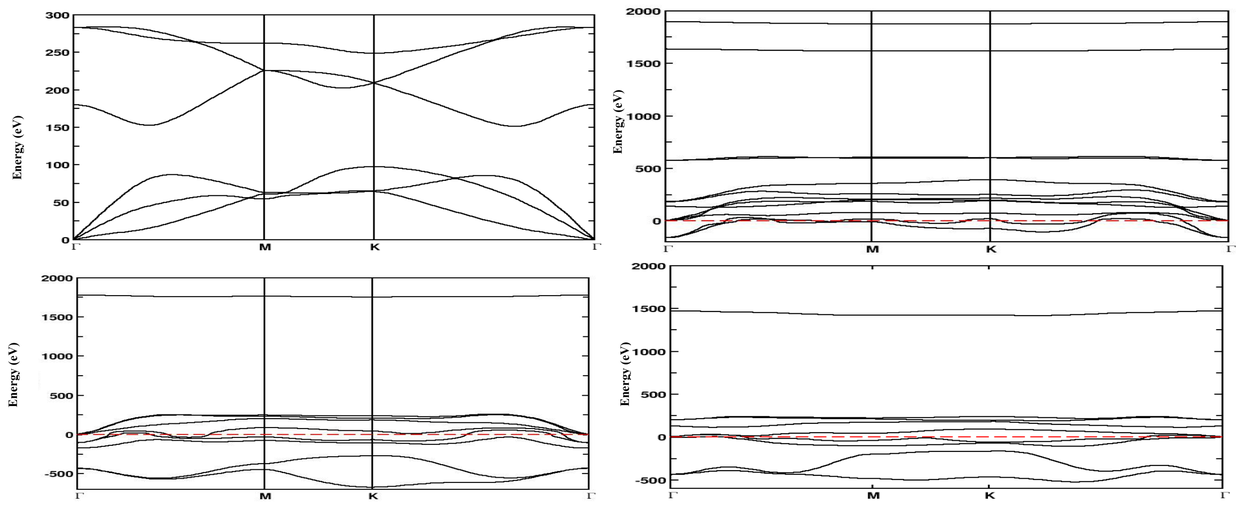

Figure 3. Phonon spectra of three models adsorpted hydro.

- Fully hydro-adsorpted have zero band gap structure like germanene. Semi adsorpted germanene behaved like metal.
- For phonon spectra, the transverse ascoustical phonon branch have imaginary energies near Γ point ⇒ dynamic unstable structure.

4. CONCLUSION

- The photoelectric properties of material have been specifically research
- The four structure maintained hexagonal symmetry and FH have the largest bonding length between Ge-Ge atom
- The phonon spectra of T2 showed that it can be executable for hydro de-sorpted process due to the dynamic unstable.