

## CHAPTER V

### CONCLUSIONS

In the present theoretical study, the molecular mechanisms of hydrogen release from borane amine ( $\text{BH}_3\text{NH}_3$ ), alane amine ( $\text{AlH}_3\text{NH}_3$ ), borane phosphine ( $\text{BH}_3\text{PH}_3$ ) and alane phosphine ( $\text{AlH}_3\text{PH}_3$ ) in systems with and without the borane ( $\text{BH}_3$ ), ammonia ( $\text{NH}_3$ ), alane ( $\text{AlH}_3$ ) and phosphine ( $\text{PH}_3$ ) were theoretically investigated by the MP2/6-311++G(d,p) and B3LYP/6-311++G(d,p) calculations. Each system, we were able to locate three different transition-state structures for hydrogen elimination with borane ( $\text{BH}_3$ ), ammonia ( $\text{NH}_3$ ), alane ( $\text{AlH}_3$ ) and phosphine ( $\text{PH}_3$ ) present. We can determine the details of each system as follows:

- For borane amine system, the activation energies in the catalytic pathway for hydrogen release from borane amine with the presence of borane ( $\text{BH}_3$ ) and ammonia ( $\text{NH}_3$ ) as the catalyst are 23.62 and 30.30 kcal/mol, respectively. But the alane ( $\text{AlH}_3$ ) and phosphine ( $\text{PH}_3$ ) molecule cannot serve as catalyst in the hydrogen elimination reactions of  $\text{BH}_3\text{NH}_3$  system.
- For alane amine system, only  $\text{NH}_3$  can play the role of a catalyst for hydrogen release from alane amine, the activation energy is 24.52 kcal/mol, but  $\text{BH}_3$ ,  $\text{AlH}_3$  and  $\text{PH}_3$  cannot act as catalyst in this system.
- For borane phosphine system, the activation energy in the catalytic pathway for hydrogen elimination from borane phosphine with  $\text{AlH}_3$  is 21.34 kcal/mol. The  $\text{BH}_3$ ,  $\text{NH}_3$  and  $\text{PH}_3$  cannot act as catalyst in this system.
- For alane phosphine system,  $\text{NH}_3$  can play the role of a catalyst for hydrogen release, the activation energy is 28.26 kcal/mol but  $\text{BH}_3$ ,  $\text{AlH}_3$  and  $\text{PH}_3$  cannot act as catalyst in this system.

- From four systems of hydrogen release reactions, the calculated results demonstrate that the  $\text{BH}_3$  and  $\text{AlH}_3$  can play the role of a most efficiency in the hydrogen release from  $\text{BH}_3\text{NH}_3$  and  $\text{BH}_3\text{PH}_3$  systems, respectively. For the  $\text{NH}_3$  can act as a most efficiency catalyst in the hydrogen release from  $\text{AlH}_3\text{NH}_3$  and  $\text{AlH}_3\text{PH}_3$  systems. But the  $\text{PH}_3$  does not behave as a catalyst. As the  $\text{PH}_3$  is the soft base, its hydrogen atoms dislike to be abstracted. Due to the large size of the  $\text{PH}_3$ , its molecular structure may destabilize the transition state of their hydrogen release reactions.
- All computational results obtained by the B3LYP/6-311++G(d,p) are in good agreement with by the MP2/6-311++G(d,p).

### **Suggestion for future work**

The hydrogen storage compounds  $\text{BH}_3\text{NH}_3$ ,  $\text{AlH}_3\text{NH}_3$ ,  $\text{BH}_3\text{PH}_3$  and  $\text{AlH}_3\text{PH}_3$  in reaction with  $\text{BH}_3$ ,  $\text{NH}_3$  and  $\text{AlH}_3$  catalysts studied in this work were found to be developed as the hydrogen energy resource. Dimers of hydrogen storage compounds studied in this work as  $(\text{BH}_3\text{NH}_3)_2$ ,  $(\text{AlH}_3\text{NH}_3)_2$ ,  $(\text{BH}_3\text{PH}_3)_2$  and  $(\text{AlH}_3\text{PH}_3)_2$  and their polymers are suggested to be studied for their hydrogen release abilities using the theoretical calculations.