

**INFORMATION**  
**ON NEW CONTRIBUTIONS OF THE DOCTORAL THESIS**  
(Information will be posted on the Website)

Title: A quantum chemical research of structure and aromaticity of some boron clusters

Major: Theoretical and Physical Chemistry. Code No: 9440119.

PhD student: Duong Van Long

Course: 06

Advisors:

1. Assoc. Prof. Dr. Nguyen Phi Hung
2. Prof. Dr. Nguyen Minh Tho

Training institution: **Quy Nhon University**

**NEW CONTRIBUTIONS OF THE THESIS**

1. Verify the suitability of the theoretical level TPSSh/6-311+G(d) for investigating the geometric structure of clusters containing B.
2. Elucidate the stability of  $B_2Si_3^q$  and  $B_3Si_2^p$  clusters using the ribbon model and Hückel rule.
3. The electron counting rules  $(4N+2M)$  and  $(4N+2M-2)$  are introduced for the disk model in the dissertation.
4. The dissertation presents a mixed disk-cone model to explain the electron configuration of cone-like clusters. The  $B_{12}Li_8$  cluster is discovered with high hydrogen storage capacity.
5. The stability of the  $B_{14}FeLi_2$  cluster is rationalized by the hollow cylinder model.


**On behalf of advisors**



Nguyen Phi Hung

*Binh Dinh, day 20 month 10 year 2023*

**PhD student**



Duong Van Long