THEORETICAL INVESTIGATION ON THE EFFECT OF CLUSTER SIZE AND LEVEL OF DENSITY FUNCITONALS IN BONDING CASE STUDY ON GLYCINE AND CYTIDINE

ABDUL RAZAK BIN MUHAMMAD

Final Year Project Report Submitted in
Partial Fulfilment of the Requirements for the
Degree of Bachelor of Science (Hons) Physics
in the Faculty of Applied Sciences
Universiti Teknologi Mara

July 2025

This Final Year Project Report entitled "**Theoretical Investigation on the Effect of Cluster Size and Level of Density Functionals in Bonding: Case Study on Glycine and Cytidine"** was submitted by Abdul Razak Bin Muhammad in partial fulfilment of the requirements for the Degree of Bachelor of Science (Hons) Physics, in the Faculty of Applied Science, and was approved by

Dr Ang Lee Sin
Supervisor
B.SC. (Hons.) Physics
Faculty of Applied Sciences
Universiti Teknologi MARA
02600 Arau
Perlis

Dr Siti Zulaikha Mohd Yusof
Project Coordinator
B.SC. (Hons.) Physics
Faculty of Applied Sciences
Universiti Teknologi MARA
02600 Arau
Perlis

Dr Rosyaini Affindi Zaman
Programme Coordinator
B.SC. (Hons.) Physics
Faculty of Applied Sciences
Universiti Teknologi MARA
02600 Arau
Perlis

25 JULY 2025

ABSTRACT

Theoretical Investigation on the Effect of Cluster Size and Level of Density Functionals in Bonding: Case Study on Glycine and Cytidine

This research investigated the theoretical calculation of the electron density for glycine and cytidine system using Density Functional Theory (DFT). This is because DFT offers a good balance between computational cost and accuracy for studying electron density distribution. The structure of glycine and cytidine was constructed using GaussView from a CIF file obtained from Hara et al. (2024). Topological analyses were performed using the Multiwfn program to identify bond critical points (BCPs) and compute $|V_{BCP}|/G_{BCP}$, and Vesta was used to visualise the electron density distribution. The result showed that the C-N, C-C and C-H bonds were covalent with high $|V_{BCP}|/G_{BCP}$ ratios (>2). The Valence Electron Density (VED) plots resembled the experimental curves more closely. The findings showed that the cluster size of neighbouring molecules have an impact on electron distributions, thus fulfilling the first objective. Although the two functionals used, APFD/def2tzvp and LC-BLYP/cc-pVTZ displayed similar bonding trends, LC-BLYP/cc-pVTZ results was slightly better in terms of long-range interactions, achieving the second objective. In conclusion, it has been shown in paper that cluster size does indeed influence the bonding interactions and electron density.

TABLE OF CONTENTS