# ABSTRAK

Penelitian ini menganalisis kestabilan sejumlah molekul radikal yang berinteraksi dengan atom atau molekul berdasarkan selisih energi HOMO dan LUMO ($\Delta E_{HL}$). Interaksi-interaksi tersebut terbagi menjadi tiga kasus. Kasus pertama adalah sejumlah molekul radikal berinteraksi dengan atom H, yaitu : OH + H $\rightarrow$ $H_2O$, $HO_2$ + H $\rightarrow$ $H_2O_2$, dan $NO_2$ + H $\rightarrow$ $HNO_2$. Kasus kedua adalah sejumlah molekul berinteraksi dengan atom F, yaitu: OH + F $\rightarrow$ FOH, $HO_2$ + F $\rightarrow$ $HO_2F$, dan $NO_2$ + F $\rightarrow$ $NO_2F$. Kasus ketiga adalah sejumlah molekul berinteraksi dengan molekul $CH_3$, yaitu:OH + $CH_3$ $\rightarrow$ $CH_3OH$, $NO_2$ + $CH_3$ $\rightarrow$ $CH_3NO_2$, dan COOH + $CH_3$ $\rightarrow$ $CH_3COOH$. Kestabilan molekul pada penelitian ini diwakili oleh besaran energi ikat. Hasil kalkulasi energi ikat untuk kasus pertama memberikan nilai 5,32 eV, 3,91 eV, dan 3,55 eV. Kasus kedua 2,05 eV, 1,33 eV, dan 2,39 eV. Kasus ketiga 4,09 eV, 2,69 eV, dan 4,17 eV. Nilai $\Delta E_{HL}$ untuk molekul radikal OH, $HO_2$, $NO_2$, dan COOH secara urut 6,19 eV, 4,23 eV, 1,47 eV, dan 2,94 eV. Kalkulasi-kalkulasi pada penelitian ini berbasis *Density Functional Theory*(DFT) menggunakan perangkat lunak Gaussian09. Hasil penelitian menunjukkan bahwa kestabilan molekul radikal memiliki pola, yaitu semakin besar $\Delta E_{HL}$ semakin besar pula energi ikat. Pola tersebut berlaku jika HOMO molekul setelah berinteraksi hanya dikonstruksi oleh HOMO molekul radikal.

**Kata kunci**: Molekul radikal, Energi ikat, selisih energi HOMO dan LUMO, dan Density Functional Theory.

# ABSTRACT

This research analyzes the stability of several radical molecules which interact with atoms or molecules based on the energy difference between HOMO and LUMO ($\Delta E_{HL}$). The interactions are divided into three cases. The first case is several radical molecules interacting with H atom, namely: OH + H $\rightarrow$ $H_2O$, $HO_2$ + H $\rightarrow$ $H_2O_2$, and $NO_2$ + H $\rightarrow$ $HNO_2$. The second case is several molecules interacting with F atom, namely: OH + F $\rightarrow$ FOH, $HO_2$ + F $\rightarrow$ $HO_2F$, dan $NO_2$ + F $\rightarrow$ $NO_2F$. The third case is several molecules interact with CH3 molecule, namely: OH + $CH_3$ $\rightarrow$ $CH_3OH$, $NO_2$ + $CH_3$ $\rightarrow$ $CH_3NO_2$, dan COOH + $CH_3$ $\rightarrow$ $CH_3COOH$. The molecular stability in this study is represented by the amount of binding energy. The results of the binding energy calculation for the first case gave 5.32 eV, 3.91 eV, and 3.55 eV respectively. The second case gave 2.05 eV, 1.33 eV, and 2.39 eV respectively. The third case gave 4.09 eV, 2.69 eV, and 4.17 eV respectively. The value of $\Delta E_{HL}$ for radical OH, HO2, NO2, and COOH molecules is 6.19 eV, 4.23 eV, 1.47 eV, and 2.94 eV, respectively. The calculations in this research are based on Density Functional Theory (DFT) using Gaussian09 software. The results showed that the stability of radical molecules has a pattern, which is higher $\Delta E_{HL}$ the higher the binding energy is. The pattern applies if HOMO molecules after interacting are only constructed by HOMO radical molecules.

**Keywords**: Radical molecules, Binding energies, Energy difference between HOMO and LUMO, and Density Functional Theory.