Electron structure on Ni_aCo_b ($2 \leq a+b \leq 6$) cluster catalyst for pyrolysis

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Catalysis is a science at the interface between chemistry, physics, biology, engineering and material sciences that enables chemical processes to be realized in a cost-, energy- and eco-efficient manner. More than 85% of the processes in the chemical industry, worth approximately € 1,500 billion annually, depending on catalytic technologies. Metal catalysts still attract many scientists' research attention due to their hydrogenate reaction. In addition, the electron structure will influence the catalyst activity, but only a few literature reports exist. The final goal of this research is to design and prepare nickel and cobalt based metal clusters (open shell and closed shell) to understand how the electron structure impacts catalyst activity related to the chemical composition of the pyrolyzed bio-oil.

Materials simulation calculations were carried out using Gaussian 16 software to design a stable catalyst cluster. The data of structural energies and Gibbs energies are shown in Figure 1 and listed in Table 1. In Figure 1, the structural energy of the Ni_aCo_b clusters is plotted versus Co atom substitution, which indicates that the total structures will decrease when the number of Co atoms increases, we observe the same effect for the Gibbs energy. In Table 1, Gibbs energy and ΔG of Ni_aCo_b ($2 \leq a+b \leq 6$) cluster are listed versus different sums of a plus b. This congruent relationship is found in references [1-2]. The higher the structurale energies, the higher the Gibbs energies. At the same time, ΔG is related to its electron structure. The open shell structures(*) always have larger ΔG, than closed shell structures, which impacts stablity and facilitates easy decomposition.

After analyzing the data, the stable catalyst compositions will be prepared by the sol-gel method, in order to verify the theoretical results. Then, we find the influence of the closed shell and open shell to the catalyst. Finally, the catalyst will be used in a fluidized bed. This reactor will be used to test catalyst activity on the pyrolized bio-oil. The relationship between the simulated catalyst structure, especially the electron structure, catalyst characterization results, and the bio-oil composition will be explained.

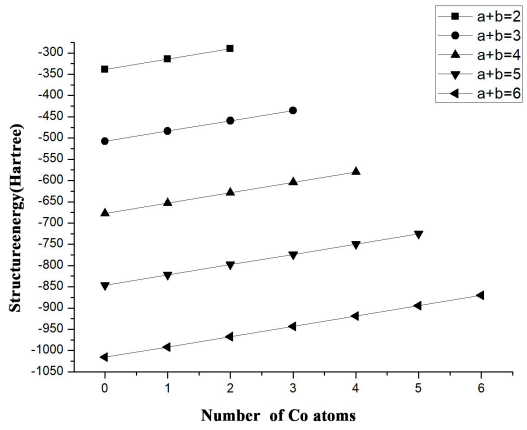

Figure 1. structure energy of Ni_aCo_b ($2 \leq a+b \leq 6$) cluster

Table 1. Gibbs energy and ΔG of Ni_aCo_b ($2 \leq a+b \leq 6$) cluster(* means open shell structure)

Name	Gibbs energy(a.u.)	ΔG(Kcal/mol)
Ni_2Co*	-483.65	55.28
$NiCo_2$	-459.42	25.28
$NiCo_3$*	-604.53	49.39
Ni_2Co_2	-628.59	-26.55
Ni_2Co_3*	-773.83	62.65
Ni_3Co_2	-797.89	-62.62
Ni_3Co_3*	-943.16	78.07
Ni_4Co_2	-967.20	-79.92

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