# DFT Study of Bimetallic Perovskite Catalysts for Steam Reforming of Bio-oil Model Oxygenates

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## ABSTRACT

Metal oxides have exhibited remarkable catalytic performance towards bio-oil steam reforming (SR) processes. Moreover, perovskite oxide ($ABO_3$) catalysts are promising owing to its combined impact of oxygen vacancies generated at A position (Lanthanide materials) and strong catalytic activity at B position (transition metals) correspondingly. In the present study, adsorption energies and their modes had been investigated to understand the catalytic trend for the SR reaction on the surface of three variant perovskite catalysts ($LaNiO_3$ (001), $LaNi_{0.8}Co_{0.2}O_3$ (001), and $LaNi_{0.8}Fe_{0.2}O_3$ (001)) using density functional theory (DFT). Furthermore, adsorption of primary bio-oil model oxygenates, steam, and key intermediates were studied on periodic slabs of perovskite catalysts. The synergistic effect of the bimetallic catalyst leads to variation in adsorption energies and enables an understanding of the relatively better catalytic behavior. The findings indicate that energies are sensitive to molecular orientation as well as surface interaction. Additionally, aromatic compounds like phenol, furfural, and benzaldehyde have more stable adsorption as compared to other molecules. On the other hand, CH was found as the major precursor for carbon deposition on the surface of perovskite catalysts because of its highest binding energy with catalyst surface. $LaNi_{0.8}Fe_{0.2}O_3$ (001) has shown the highest adsorption energy and shorter bond length of bio-oil model compounds and steam, while $LaNi_{0.8}Co_{0.2}O_3$ (001) possesses optimum energy and bond length values for all the investigated molecules. The binding energy for bio-oil model oxygenates and steam reduces in the following order: $LaNi_{0.8}Fe_{0.2}O_3$ (001) > $LaNi_{0.8}Co_{0.2}O_3$(001) > $LaNiO_3$ (001). Therefore, this study confirms that the cobalt doped $LaNiO_3$ (001) catalyst is the most efficient among the three distinct perovskites investigated for its optimal values of molecular binding.

**Keywords:** Hydrogen production; Density Functional Theory Study; Bio-oil model oxygenates; Steam Reforming; Perovskite catalyst.

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