

Computational investigation of the Co-support interfaces on γ -Al₂O₃, SiO₂ and TiO₂

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Despite its history spans over almost a century, the Fischer-Tropsch process has recently gained renewed interest from the scientific community in light of its potential to speed-up the energy transition. In fact, by converting syngas into a wide variety of hydrocarbon products, this technology makes it possible to produce fundamental chemical commodities from renewable feedstocks.

Supported cobalt catalysts are particularly suitable for the Fischer-Tropsch synthesis as they showcase high activity under mild process conditions, with operating temperatures usually not exceeding 493 K. The interactions between Co and the support prominently affect the performance of the catalyst, as they largely control Co dispersion and reducibility [1]. Nonetheless, due to the complexity of these systems, it is often arduous to univocally resolve the nature of the metal-support interactions based solely on experimental observations, and, as a result, a consensus on the phenomena governing the formation of the Co-support interfaces is largely missing.

In this work, DFT calculations at the GGA+U level of theory were employed to gain molecular understanding of the conformation of the interfaces between Co and three of the most widely employed supports, namely γ -Al₂O₃, SiO₂ and TiO₂. It was found that, while TiO₂ displays reasonable chemical affinity with metallic cobalt, for SiO₂ and especially γ -Al₂O₃ the existence of an intermediate oxidic layer that glues together Co⁰ and the support must be postulated to explain the adhesion between the two materials. On alumina, this intermediate layer can form readily and ensures strong adhesion of Co⁰ everywhere on the support, promoting high cobalt dispersion. On SiO₂, the formation of the oxidic glue is less favored and is expected to strongly depend on the synthesis procedure; additionally, strong adhesion is only possible on specific anchoring sites with low concentration of surface silanols such as defects.

References

- [1] G. Jacobs, T. K. Das, Y. Zhang, J. Li, G. Racoillet, B. H. Davis, *Applied Catalysis A: General* **233** (2002)