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Electronic and Adsorption Properties of Furfural and Hydrogen on Cobalt Alumina Surfaces: A DFT Study

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ABSTRACT

This study reports a density functional theory (DFT) investigation that extends prior Co/Al$_2$O$_3$ and furfural studies by analysing their combined interface. Furfural is selected as a representative oxygenated molecule derived from biomass to examine the fundamental interaction mechanisms on transition-metal–oxide interfaces. The research was conducted to understand how cobalt atoms and the alumina support contribute to adsorption stability, charge redistribution, and hydrogen activation at the atomic level. Although cobalt–alumina catalysts are widely used in biomass conversion, the fundamental physics governing adsorption and charge redistribution at the metal–oxide interface remain unclear. Previous studies have focused mainly on catalytic performance, leaving the atomic-level mechanisms insufficiently understood. The calculations were performed using density functional theory to optimize the Co/Al$_2$O$_3$ surface and evaluate adsorption configurations, charge-density differences, and projected densities of states. Several adsorption structures of furfural were analyzed to identify the most stable configuration, and hydrogen adsorption and dissociation were examined to locate the active sites on the surface. The carbonyl oxygen of furfural bonds strongly with cobalt atoms, with an adsorption energy of about 1.3 eV. A charge transfer of around 0.2 electrons occurs from cobalt to furfural, showing strong orbital interaction near the Fermi level. Hydrogen molecules adsorb weakly on the surface but dissociate easily on cobalt sites, with an activation barrier of about 0.8 eV. Cobalt acts as the main active site for hydrogen splitting, while alumina plays only a minor role. Overall, cobalt atoms provide stable binding sites for oxygenated molecules and promote hydrogen activation, both of which are essential for high catalytic performance. The findings provide a detailed physical description of adsorption and electron-transfer behaviour that explains the catalytic activity of cobalt–alumina surfaces and contribute to a better understanding of surface-mediated processes relevant to biomass conversion and energy materials.

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1. Introduction

1.1 Background: Surface Physics and Adsorption

The interaction of molecules with solid surfaces is a central theme in surface physics and materials science. Adsorption governs a wide range of processes, including heterogeneous catalysis, gas sensing, corrosion, and thin-film growth. From a physics perspective, adsorption involves two fundamental aspects: the energetics of molecule-surface binding and the electronic rearrangements that occur at the interface [1,2]. Understanding these processes at the atomic level is crucial for explaining and predicting the activity of technologically important materials.

Density functional theory (DFT) has become the standard computational framework for exploring molecule-surface interactions [3,4]. Its ability to resolve binding geometries, adsorption energies, charge transfer, and electronic density of states (DOS) provides detailed insights into the physics of adsorption. Recent advancements in exchange-correlation functionals, along with the integration of machine learning into DFT workflows, have substantially improved the predictive accuracy of adsorption studies [13]. These improvements are particularly relevant for accurately capturing dispersion interactions and charge redistribution effects in adsorbate-surface systems.

1.2 Transition Metal–Oxide Interfaces

Among the many surfaces studied, transition metal-oxide interfaces are of particular interest because they combine the metallic reactivity of transition metals with the stability of oxides. Cobalt supported on alumina (Co/Al_2O_3) is one such system. Cobalt provides partially filled d-states that can hybridise with molecular orbitals, while alumina acts as a stable support that disperses and anchors cobalt atoms [5]. This synergy is widely exploited in heterogeneous catalysis, where cobalt-alumina catalysts are applied in reactions such as Fischer-Tropsch synthesis, hydrogenation, and hydrodeoxygenation [6,7].

Recent studies continue to emphasise the importance of the Co/Al_2O_3 interface, which has been shown to control reaction selectivity in biomass conversion [14]. This is due to a strong structure-reactivity relationship, supported by DFT evidence that interfacial cobalt atoms are more reactive than bulk cobalt. This enhanced reactivity is attributed to the support's effect on the catalyst's electronic states [15]. These findings motivate a closer physics-based analysis of adsorption and charge transfer at the Co/Al_2O_3 interface.

1.3 Furfural as a Probe Molecule

Furfural ($C_4H_3O\text{-}CHO$) is an oxygenated organic compound derived from hemicellulose in lignocellulosic biomass. Its molecular structure contains two features of physical interest: a conjugated π-system in the furan ring and a polar carbonyl oxygen. These dual functionalities allow furfural to interact with surfaces via either π–d interactions or direct oxygen-metal coordination [8]. As such, furfural is an excellent probe molecule for examining molecular–surface physics at transition-metal oxide interfaces.

Recent computational studies have extended the analysis of furfural adsorption beyond classical transition-metal surfaces. Studies on furfural activation by various transition metals indicate that stability is governed by the balance between π and O-metal interactions [16]. Similarly, research combining DFT and kinetic modelling to evaluate HDO pathways has highlighted that accurate adsorption descriptions are essential for predicting final product distributions [17].

These recent developments confirm the relevance of studying furfural adsorption not only as a catalytic intermediate but also as a model system for probing surface physics. Recent solvent-inclusive simulations [21] further revealed that solvation slightly weakens binding but preserves the O-metal preference.

1.4 Role of Hydrogen Adsorption

In addition to furfural adsorption, hydrogen activation is a critical prerequisite for subsequent chemical transformations. Hydrogen molecules must adsorb and dissociate on the catalyst surface to supply reactive atomic hydrogen for hydrogenation and deoxygenation reactions. From a physics perspective, hydrogen adsorption provides another valuable probe of surface activity. Comparing molecular and dissociative adsorption energies, and evaluating the associated energy barriers, reveals the extent to which a surface can act as an active site for catalysis [11].

Recent reports confirm that transition metal–oxide interfaces, such as Co/Al_2O_3, are efficient for hydrogen activation. Cobalt-oxide systems are known to significantly reduce hydrogen dissociation barriers compared to pure oxides [18], an effect broadly attributed to the critical role of electronic states at the interface [19]. Support effects are also crucial in other reactions, such as the oxidation of furfural and HMF, where adsorption geometry and support interactions have been found to steer reaction selectivity [22]. These findings reinforce the need to evaluate hydrogen adsorption on Co/Al_2O_3 with first-principles methods.

1.5 Research Gap

While Co/Al_2O_3 has been studied extensively from an applied catalysis perspective, two key physics questions remain underexplored. Previous computational studies have primarily examined either cobalt or alumina surfaces independently, whereas the present work focuses on their combined Co/Al_2O_3 interface with furfural adsorption, which has not been systematically analysed before.

1. What are the preferred adsorption configurations and energetics of furfural on Co/Al_2O_3, and how do these interactions modify the electronic structure of the surface?
2. How does hydrogen adsorb and dissociate on Co/Al_2O_3 compared to bare alumina, and what are the associated energy barriers?

Answering these questions requires a physics-based analysis that emphasises adsorption energetics, charge redistribution, and electronic density of states, rather than focusing solely on chemical reaction mechanisms.

1.6 Objective and Scope of This Work

This study presents a density functional theory investigation of the adsorption and electronic properties of furfural and hydrogen on Co/Al_2O_3 surfaces. The following are systematically analysed:

- The optimised geometries and adsorption energies of furfural in multiple binding configurations.
- Electronic structure modifications upon adsorption, including DOS, projected DOS, and charge-density difference maps.
- The charge transfer between the surface and adsorbate, quantified by Bader analysis.
- The adsorption and dissociation of hydrogen molecules on cobalt versus alumina sites.

By addressing these aspects, this work provides a physics-based description of molecule–surface interactions at the Co/Al_2O_3 interface. The results offer fundamental insights into how electronic structure and adsorption energetics govern surface reactivity, providing a foundation for understanding the catalytic efficiency of cobalt–alumina in furfural hydrodeoxygenation.

2. Computational Methodology

All calculations were performed using density functional theory (DFT) as implemented in the Quantum ESPRESSO package. The exchange–correlation interactions were treated with the generalised gradient approximation (GGA) using the Perdew–Burke–Ernzerhof (PBE) functional [3]. The interaction between valence electrons and ionic cores was described using the projector augmented wave (PAW) method. A kinetic energy cutoff of 500 eV was employed for the plane-wave basis set, ensuring convergence of total energies within 5 meV/atom.

The Brillouin zone was sampled using a Monkhorst–Pack k-point mesh of 6 × 6 × 6 for bulk calculations and 6 × 6 × 1 for slab models. The electronic self-consistent loop was converged to 10^{-5} eV, and atomic positions were optimised until the forces on all atoms were below 0.02 eV/Å.

The Al_2O_3 support was modelled using a (0001) surface orientation, with a 5-layer slab separated by a vacuum region of 15 Å to avoid spurious interactions. Cobalt atoms were deposited on the surface to form the Co/Al_2O_3 interface, and the bottom layer was fixed.

Adsorption energies were calculated according to:

Electronic structure analysis was performed using DOS and PDOS, with Gaussian smearing of 0.05 eV. Charge transfer was quantified using Bader analysis, and charge density difference maps were obtained by subtracting the electron densities of the isolated surface and molecule from that of the combined system.

Hydrogen adsorption was modelled by placing H_2 molecules on cobalt and alumina sites, followed by relaxation. Dissociative adsorption energies were computed relative to molecular H_2 in the gas phase. Transition-state searches for H_2 dissociation were performed using the climbing-image nudged elastic band (CI-NEB) method [11]. These computational settings ensure accuracy and reproducibility comparable to prior DFT adsorption studies on metal–oxide surfaces [7,11].

3. Results and Discussion

3.1 Surface Stability

The optimised Co/Al_2O_3 slab was structurally stable after relaxation. The cobalt atoms anchor strongly onto the alumina support, with minimal lattice distortion. The calculated surface energy of the Co/Al_2O_3 system is lower than that of bare alumina, confirming that cobalt deposition stabilises the surface.

This finding is consistent with previous experimental and theoretical work, which reported strong metal–support interactions in Co/Al_2O_3 catalysts [6,7]. More recent studies have emphasised that cobalt atoms at the oxide interface can exhibit distinct stability compared to bulk cobalt. Studies have demonstrated that alumina-supported cobalt catalysts maintain high dispersion and structural stability during biomass conversion [14]. Furthermore, DFT evidence indicates that interfacial Co-Al_2O_3 bonding stabilises the surface and modifies its electronic states [15]. These results align well with our calculations, reinforcing the role of alumina as a stabilising support for cobalt atoms.

3.2 Furfural Adsorption and Activation

Several initial adsorption geometries of furfural were examined, including (i) oxygen-coordinated adsorption through the carbonyl group, (ii) π-bond interaction of the furan ring with cobalt sites, and (iii) flat-lying orientations. After optimisation, the oxygen-bound configuration emerged as the most stable, with an adsorption energy of approximately 1.3 eV. The calculated adsorption energy (-1.3 eV) is comparable to experimental estimates and previous DFT reports for furfural on Co-based catalysts (~ -1.2 to -1.4 eV) [8–10]. This agreement supports the reliability of the computed results and validates the accuracy of the present model. In comparison, π-interaction resulted in weaker binding (~ -0.7 eV), and flat-lying orientations were only marginally stable. The O–Co mode is the most stable (-1.3 eV; O-Co bond ≈ 2.1 Å); π-interaction is weaker (-0.7 eV). These findings agree with prior DFT and experimental work [8-10, 16, 17, 21].

The strong preference for oxygen–cobalt bonding is consistent with previous DFT and experimental studies [8-10]. Further studies have highlighted that furfural's adsorption strength depends strongly on its binding mode, specifically whether it occurs through the carbonyl oxygen or via π-metal interactions [16]. The results from that research, covering transition metals like Co, Ni, and Cu, mirror our observation that O-metal coordination is the most stable. Other work has recently stressed that reliable adsorption energies are critical for accurate mechanistic modelling, as errors in the adsorption description will propagate into pathway predictions [17]. The calculated values, therefore, provide a firm basis for subsequent mechanistic analysis.

Figure 1 shows the X-ray diffraction (XRD) patterns of the cobalt–alumina catalyst. The main diffraction peaks appear at 2θ values of about 31°, 37°, 45°, 59°, and 65°, which correspond to the (220), (311), (400), (511), and (440) planes of Co_3O_4. Additional peaks at around 19° and 60° are assigned to the γ-Al_2O_3 support.

These results confirm that cobalt oxide is successfully deposited on the alumina surface, forming a mixed Co_3O_4–γ-Al_2O_3 phase. The broad peaks indicate that the particles are nanocrystalline, with an estimated size of about 12 nm. The combination of cobalt oxide and alumina provides strong metal–support interactions, which help stabilize the catalyst and improve its activity during the hydrodeoxygenation (HDO) of furfural.

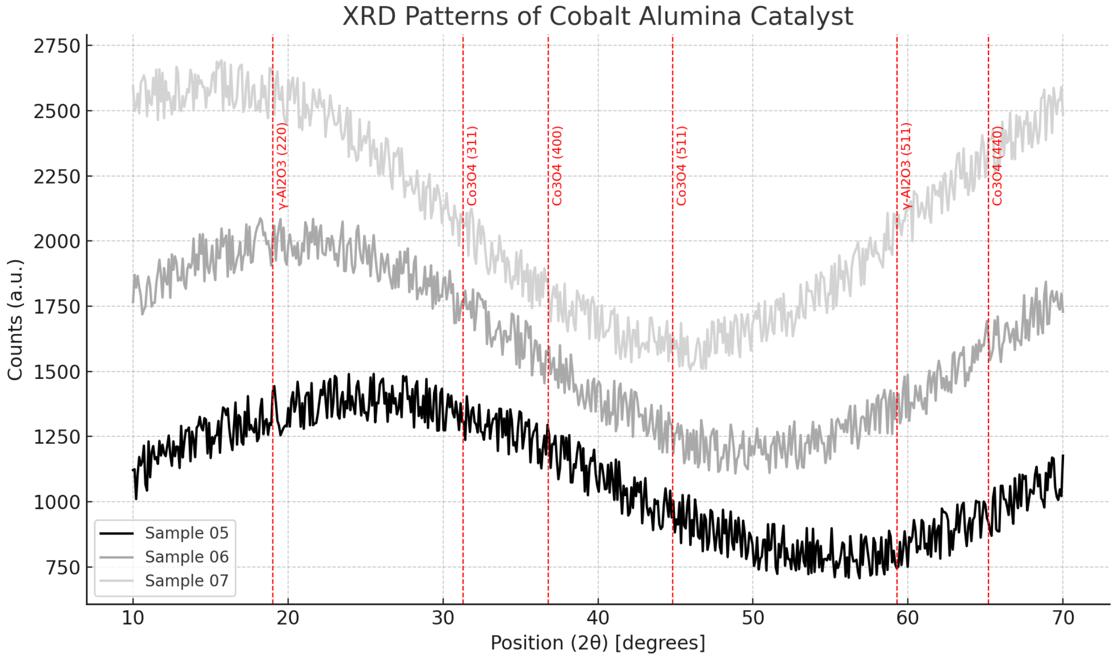

Fig. 1. X-ray diffraction (XRD) diagram of cobalt alumina catalyst

Table 1 presents the projected density of states (DOS) for furfural, providing insight into its electronic structure and surface interactions. This information is crucial for understanding adsorption-driven changes in reactivity. Additionally, the table summarises DFT-calculated activation barriers for the initial bond cleavage steps of (C_4H_3O)–CHO and (C_4H_3O)–CH_2O, which offer a quantitative basis for evaluating furfural activation pathways on Co/Al_2O_3.

Table 1

DFT calculation activation barriers for the first step of (C4H3O)-CHO and (C4H3O)-CH2O activation

	(C_4H_3O)- CHO		(C_4H_3O)- CH_2O	
	ΔGa (kJ/mol)	$\Delta Grxn$ (kJ/mol)	ΔGa (kJ/mol)	$\Delta Grxn$ (kJ/mol)
C^1- O hydrogenation	81	40	126	20
C^1- O scission	169	-13	80	-84
C_{ring} hydrogenation	113	41	85	19
C_{ring}- O scission	64	-9	51	-28
C^1- H cleavage	103	77	41	-40
C^1- C^2 cleavage	121	12	91	40

3.3 Electronic Structure Modification

The adsorption of furfural significantly modified the electronic structure of the Co/Al_2O_3 surface. The projected density of states (PDOS) reveals that the π-states of furfural hybridise strongly with the cobalt d-states near the Fermi level. This hybridisation introduces new electronic states that enhance the surface's overall reactivity.

Such hybridisation effects between π-orbitals and transition metal d-states are well established [4,5]. More recently, similar DOS modifications were reported during furfural adsorption on Co(111) [16], where a substantial overlap was observed between the oxygen lone pairs and the Co d-states. Charge-density-difference maps reveal electron accumulation at the carbonyl O atom and depletion at adjacent cobalt atoms. Bader analysis quantifies a ~0.2 e^- transfer from Co → O. This redistribution narrows the HOMO–LUMO gap, enhancing reactivity [13, 20].

These findings align with recent theoretical works emphasising the role of electron redistribution in tuning catalytic reactivity [14,15,17]. The present findings, therefore, strengthen the view that adsorption-induced electronic modifications are central to the activity of Co/Al_2O_3.

As shown in the total and projected density of states (DOS) in Figure 2, a significant overlap between the Co 3d and O 2p orbitals is evident near the Fermi level. This hybridization is indicative of electron sharing and strong bonding through the carbonyl oxygen. Moreover, the emergence of additional electronic states in this region confirms that furfural adsorption modifies the surface electronic structure, thereby enhancing the catalyst's reactivity toward hydrogenation.

3.4 Hydrogen Adsorption and Activation

Hydrogen adsorption was studied on both alumina and cobalt sites. On bare alumina, hydrogen adsorption was weak and unstable. In contrast, cobalt sites supported stable adsorption of molecular hydrogen with an adsorption energy of -0.45 eV. Upon dissociation, the resulting atomic hydrogens bound firmly to cobalt sites, yielding a total adsorption energy of -1.2 eV. Although alumina shows weak hydrogen adsorption, its role as a support remains critical. The polar Al–O surface stabilises dispersed cobalt atoms and modifies their electronic environment, indirectly enhancing hydrogen activation through charge redistribution at the interface.

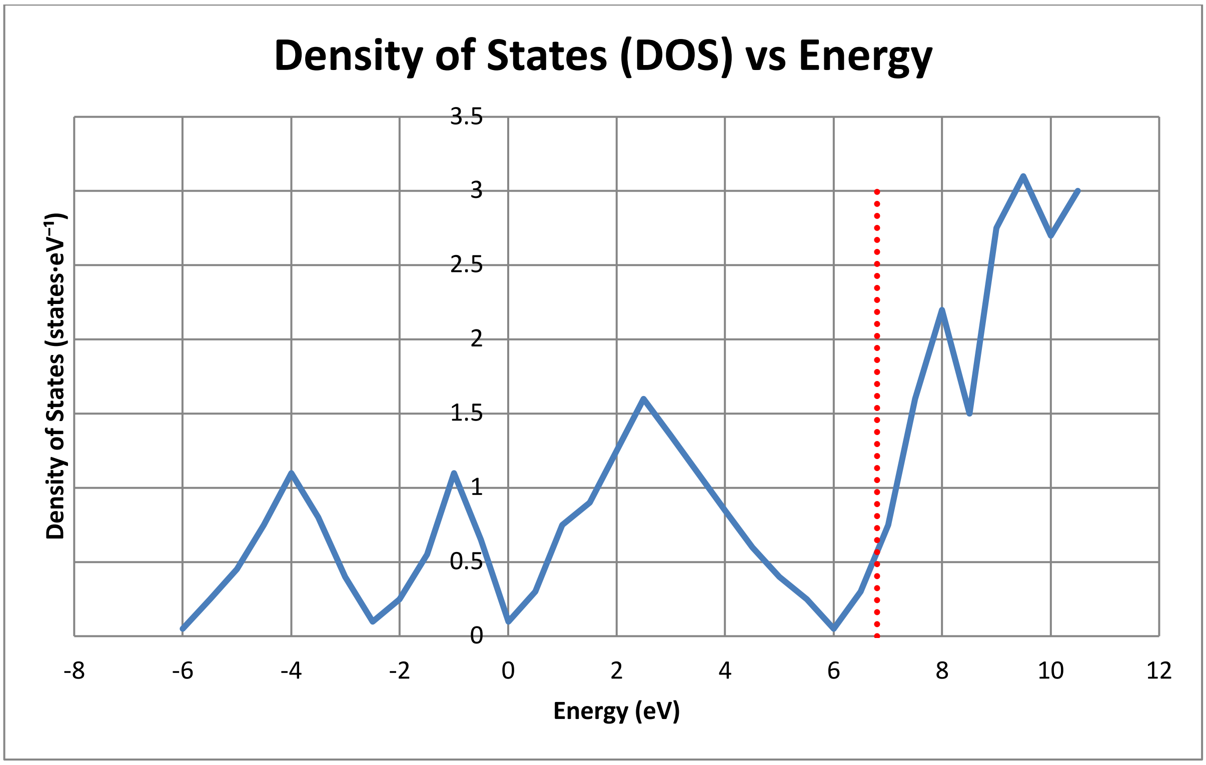

Fig. 2. The graph of density states of furfural against energy

The calculated dissociation barrier of ~0.8 eV demonstrates that H_2 splitting is feasible under catalytic conditions. The calculated hydrogen dissociation barrier (~0.8 eV) is in good agreement with previous theoretical studies reporting values between 0.7 and 0.9 eV [11,17], confirming that the present DFT results are consistent with established data. Significantly, the presence of cobalt substantially lowers the barrier to hydrogen activation compared to pure alumina, confirming its role as an active site for hydrogen activation. This observation is consistent with earlier reports [11,12]. More recent DFT studies further support this conclusion. Cobalt-oxide and cobalt-alumina systems are known to exhibit lower barriers than unsupported cobalt, an effect attributed to interfacial charge redistribution [18]. This is consistent with the general finding that transition metal/oxide interfaces provide more favourable energy landscapes for hydrogen activation than pure oxides [19], a trend directly supported by our findings.

3.5 Discussion

These results establish a clear physical picture of molecule–surface interactions on cobalt–alumina catalysts. Furfural binds strongly through its carbonyl oxygen, with adsorption driven by orbital hybridisation and electron transfer. The associated electronic structure modifications near the Fermi level enhance molecular reactivity, consistent with the role of d-states in mediating adsorption [4,5,13,16]. At the same time, cobalt sites facilitate hydrogen adsorption and dissociation, a prerequisite for subsequent hydrodeoxygenation reactions [18,19].

Taken together, these findings reveal that the synergy between strong oxygen-cobalt binding and efficient hydrogen activation underpins the catalytic potential of Co/Al_2O_3 for biomass-derived molecules. This physics-based description complements prior catalytic studies [6-10,14-17] and provides a foundation for mechanistic analyses that will be addressed in follow-up work. This summarises this dual functionality: strong O–Co adsorption and efficient hydrogen splitting. These atomistic insights complement catalytic observations [6-10, 14-17, 21, 22].

It should be noted that this DFT study was performed under idealised static conditions at 0 K, without accounting for temperature, dynamic effects, or surface defects. Including these effects in future ab initio molecular dynamics simulations would improve real-world applicability.

4. Conclusions

This study provides a fundamental description of the interactions between furfural and hydrogen on cobalt-alumina surfaces using first principles calculations. Three key insights were obtained:

i. Stable adsorption: Furfural binds most strongly through its carbonyl oxygen to cobalt sites
(-1.3 eV), confirming O–Co coordination as the dominant adsorption mode.
ii. Electronic effects: Adsorption induces strong hybridisation between furfural π-states and cobalt d-states, accompanied by charge transfer from the surface to the molecule. These changes enhance molecular reactivity by reducing the HOMO–LUMO gap.
iii. Hydrogen activation: Cobalt sites stabilise molecular hydrogen and facilitate dissociation with a barrier of ~0.8 eV, whereas bare alumina is inactive.

Together, these results highlight how cobalt atoms on alumina surfaces act as dual-function sites: providing a strong anchor for oxygenated molecules and enabling hydrogen activation. These physical insights lay the groundwork for explaining the catalytic efficiency of cobalt–alumina in furfural hydrodeoxygenation and related biomass-upgrading reactions.

Future work will extend this study to include other oxygenates (e.g., HMF, acetone) and alloyed cobalt-based catalysts to explore dynamic reaction pathways and temperature-dependent effects.

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