

Mechanistic Understanding of Furan Hydrogenation to Tetrahydrofuran on Transition-metal Surfaces Using Density Functional Theory

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Abstract—One of the crucial processes in the upgrading of biomass and the generation of green solvents is the selective Hydrogenation of Furan to Tetrahydrofuran (THF). This study employed Density Functional Theory (DFT) to investigate the complete hydrogenation sequence of furan to THF on transition metal surfaces such as Pd (111), Pt (111), and Ni (111) surfaces. Furan adsorbs preferentially in a flat configuration at the fcc site, with binding energies of -1.74 eV, -1.91 eV, and -1.46 eV on Pd, Pt, and Ni, respectively, while THF exhibits weaker interactions (-0.95 eV, -0.85 eV, and -0.68 eV), indicating physisorption and facile desorption. Hydrogenation proceeds through four sequential steps, with site preferences varying across metals. On Pd (111), the third hydrogen addition at the α -carbon (C4) is rate-determining, with an activation barrier of 1.10 eV. On Pt (111), the third hydrogenation at the β -carbon (C2) is rate-limiting, with a barrier of 1.02 eV, whereas on Ni (111), the fourth and final hydrogenation step at the β -carbon (C3) is the slowest, with a barrier of 0.89 eV. Bader charge analysis of key transition states further elucidates how electron redistribution between the reacting carbon and hydrogen stabilizes the transition states, rationalizing the metal-dependent pathways. Although Ni (111) appears to be the most active metal based on DFT energetics, this trend does not align with experimental observations, whereas Pd (111) and Pt (111) show excellent consistency with observed selectivity and activity. Overall, the investigation presents a clear mechanistic perspective on metal-dependent reactivity and develops a DFT-based framework for connecting surface energetics to experimental selectivity trends in furan hydrogenation.

Keywords—furan, biomass conversion, Furan to Tetrahydrofuran (THF), Density Functional Theory (DFT), hydrogenation, heterogeneous catalysis

I. INTRODUCTION

The transformation of biomass into industrially relevant chemicals has gained significant attention due to the global movement toward carbon-neutral innovations and rising concerns about the diminishing reserves of petroleum [1, 2]. Furanic compounds produced by lignocellulosic biomass, in particular, show strong potential as renewable feedstocks because of their diverse chemical activity. One of the most important furanic molecules, furan, can be hydrogenated to produce various valuable derivatives. Tetrahydrofuran (THF) is a useful solvent that is widely used in the manufacture of polyvinyl chloride (PVC) and 3D printing materials, as well as other chemical synthesis processes. It also acts as a crucial intermediate in the production of pharmaceuticals and fine chemicals, emphasizing its industrial and commercial importance [3]. Fig. 1 illustrates the complete hydrogenation of furan to THF.

The carbon atoms in the furan ring have been designated C1–C4 to indicate the different hydrogenation steps. C1 and C4 are α -carbons, indicating they are directly adjacent to the oxygen atom, while C2 and C3 are β -carbons.

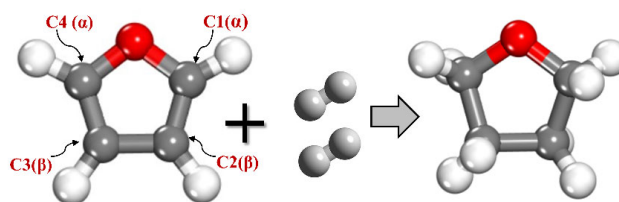


Fig. 1. Schematic representation of the Hydrogenation of Furan to Tetrahydrofuran (THF). Color code: Carbon = gray, oxygen = red, hydrogen = white.

II. LITERATURE REVIEW

The conversion of furan to THF has been investigated experimentally using supported transition-metal catalysts such as Palladium, platinum, or nickel [4–6]. However, it is essential to uncover the underlying reaction mechanism and elementary steps governing furan hydrogenation on these metal surfaces.

Density Functional Theory (DFT)-based simulations have been widely employed to investigate these mechanisms [7, 8]. Agrawal *et al.* [9] investigated the thermochemical conversion of xylose through several reaction mechanisms involving intermediates like furan and THF, offering insightful information for comprehending the furan $\rightarrow$ THF transformation. However, all reactions were investigated in the homogeneous water phase, thereby bypassing key aspects such as adsorption and metal-surface effects. Rao *et al.* [10] studied the spectroscopic constants, anharmonic force fields, and vibrational frequencies for furan using DFT-VPT2, providing vibrational data useful for validating DFT descriptors of furan and its intermediates. However, their work also focuses exclusively on gas-phase molecules and does not consider the implications of adsorption. Salnikov *et al.* [11] employed the parahydrogen-induced polarization strategy to gain mechanistic insights into the hydrogenation of furans and dihydrofurans over metal-supported catalysts. However, experimental elucidation of such mechanisms remains challenging as surface intermediates are short-lived and difficult to detect experimentally. This makes DFT-based computational investigations particularly valuable for predicting reaction pathways and energetics.

Wang *et al.* [12] used DFT to study the ring-opening and hydrogenation routes of furan on the Pd surface, with an emphasis on the formation of THF and 1-butanol. While such studies have provided valuable mechanistic insights, a systematic comparison of furan hydrogenation across different transition-metal surfaces is still lacking. Such an analysis is essential for understanding how hydrogen addition sites, intermediate stability, and metal-adsorbate interactions differ among Pd, Pt, and Ni, ultimately dictating the activity and product selectivity. To address this gap, the present study employs DFT to map the complete hydrogenation pathway of furan to THF on Pd (111), Pt (111), and Ni (111) surfaces. We identify the most favorable hydrogenation routes, compute activation barriers and intermediate stabilities, construct detailed Potential Energy Surfaces (PES) for each metal, and determine the Rate-Determining Step (RDS). This comparative framework enables a direct comparison of Pd, Pt, and Ni surfaces, providing insights for rational catalyst design aimed at enhancing activity and selectivity toward THF production.

III. COMPUTATIONAL METHODS

The Vienna Ab Initio Simulation Package (VASP) was employed for implementing the periodic plane-wave-based DFT [13]. The Perdew-Burke-Ernzerhof (PBE) functional with Grimme's D3 dispersion correction was used to treat the exchange-correlation interactions [7, 14]. The ionic cores were modeled using the Projector Augmented-Wave (PAW) approach [15, 16]. A Gaussian smearing with $\sigma = 0.20$ eV and a plane-wave energy cutoff of 400 eV was used, which has been shown to be appropriate for similar systems [12, 17]. The Self-Consistent Field (SCF) energy convergence limit was established at 10^{-5} eV, and geometry optimizations were carried out until the force criterion of 0.1 eV/Å per atom was satisfied.

The (111) surfaces of all three metals were selected as model surfaces because different studies (like XRD) have shown that the (111) facet is the most thermodynamically stable and predominantly exposed surface in face-centered cubic (fcc) transition metals [18]. Surface computations were performed using a 4×4 supercell with four atomic layers. The bottom layer remained fixed during relaxation. A vacuum thickness of 12 Å was added to avoid interactions between periodic pictures. These parameters were optimized to ensure that changes in supercell size, slab thickness, or vacuum spacing did not significantly affect adsorption energies or reaction barriers. The bulk computations used the tetrahedron approach with Blöchl [19] corrections and an $11 \times 11 \times 11$ Monkhorst-Pack k-point mesh. Surface computations were performed using a $3 \times 3 \times 1$ k-point grid to balance accuracy and cost. The Climbing-Image Nudged Elastic Band (CI-NEB) method was implemented with 6–8 intermediate structures to identify transition states along the reaction pathway [20]. A single imaginary vibrational mode, identified via harmonic frequency analysis, was used to validate the transition states.

Reaction energies (ΔE_R) and activation barriers (E_a) were estimated according to Eqs. (1) and (2). In these equations, $E_{\text{Reactants}}$, $E_{\text{Transition-state}}$, and E_{Products} represent the energies of the initial, transition, and final states (IS, TS, FS), respectively.

$$\Delta E_R = E_{\text{Products}} - E_{\text{Reactants}} \quad (1)$$

$$E_a = E_{\text{Transition-state}} - E_{\text{Reactants}} \quad (2)$$

IV. RESULTS AND DISCUSSION

A. Binding Energy of Furan and THF on 111 Surfaces

We investigated several adsorption configurations of furan and THF on (111) surfaces of Pd, Pt, and Ni. In line with earlier research, Furan has been found to adsorb at the fcc site with a planar geometry. Furan adsorbs almost parallel to the Pd (111) surface, according to Knight *et al.*'s [21] near-edge X-ray Absorption Fine Structure (NEXAFS) and Photoelectron Diffraction (PhD) studies.

The most favorable adsorption configurations of Furan and THF on the three surfaces are shown in top-view in Fig. 2, with their corresponding binding energies presented below each structure. Side views are included as insets in the upper corners to illustrate the adsorption geometries. For furan, the calculated electronic binding energy on Pd (111) is -1.74 eV (Fig. 2a). In the optimized geometry, the carbon atoms exhibit strong proximity to the surface while the oxygen atom is slightly repelled, suggesting a stronger π - π -metal interaction compared to O-metal bonding. On Pt (111), Furan exhibits a stronger binding energy of -1.91 eV (Fig. 2b), reflecting Pt's higher affinity for π -systems. In contrast, Ni (111) exhibits the weakest interaction, with a binding energy of -1.46 eV (Fig. 2c). This weaker adsorption arises from the differences in the d-band center position of Ni relative to Pd and Pt, which influences the overlap between the furan π -orbitals and the metal d-states.

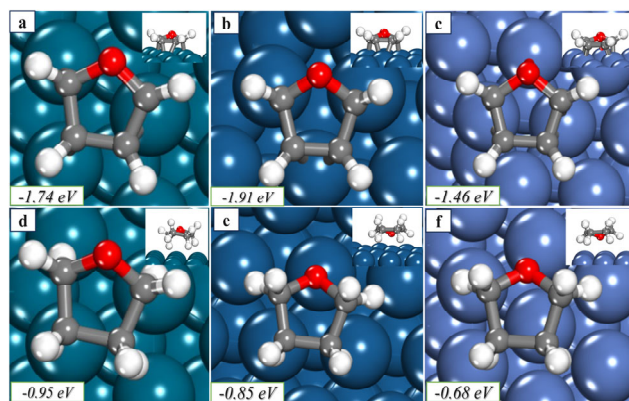


Fig. 2. Most stable adsorption configurations of furan and THF on Pd (111), Ni (111), and Pt (111) surfaces. (a) furan/Pd (111), (b) furan/Pt (111), (c) furan/Ni (111), (d) THF/Pd (111), (e) THF/Pt (111), and (f) THF/Ni (111). The corresponding electronic binding energies are shown in each subfigure, with side-view insets (upper corners). Colour code: Carbon = gray, oxygen = red, hydrogen = white, metals = teal (Pd (111)), blue (Pt (111)), violet-blue (Ni (111)).

THF, in comparison, interacts weakly with all three metal surfaces, predominantly through van der Waals forces. The stable adsorbed geometry preserves a nearly gas-phase-like conformation with slight ring deformation. On Pd (111), THF exhibits a binding energy of -0.95 eV, indicating physisorption (Fig. 2d). The interaction is weaker on Pt (111) (-0.85 eV, Fig. 2e) and weakest on Ni (111) (-0.68 eV, Fig. 2f). These relatively small adsorption energies suggest

that THF can desorb readily under reaction conditions, which is favorable for catalytic turnover. An interesting structural feature is the orientation of the oxygen atom in THF. On Pd (111), the oxygen atom experiences a slight repulsion from the surface, whereas on Pt (111) and Ni (111) the oxygen atom bends toward the surface, suggesting subtle differences in O–metal interactions across the three catalysts.

B. Reaction Mechanism

Furan is completely hydrogenated to THF in four sequential hydrogenation steps. A key mechanistic question in this process concerns the identity of the first carbon atom attacked by hydrogen: C1, C2, C3, or C4 (Fig. 1). Due to the ring's symmetry, hydrogenation at C1 and C4 are equivalent, as are hydrogenation events at C2 and C3. Thus, only two unique possibilities need to be considered in the initial step: hydrogenation at the α -carbon (C1, adjacent to the oxygen atom) and at the β -carbon (C2). On Pd (111), hydrogenation at C1 exhibits an activation barrier of 0.94 eV with a moderately endothermic reaction energy of 0.49 eV. In contrast, hydrogenation at C2 is less favorable, requiring a substantially higher barrier of 1.23 eV and a reaction energy of 0.60 eV. These results suggest that the α -carbon is the kinetically preferred site for the first hydrogenation step on Pd (111), leading to the Furan-1H* intermediate. A similar trend is observed on Pt (111) and Ni (111). On Pt (111), hydrogenation at C1 is highly favorable, with a low barrier of 0.54 eV, and the process is exothermic with a reaction energy of -0.26 eV. On Ni (111), the corresponding barrier is 0.86 eV, and the reaction is endothermic with a reaction

energy of 0.47 eV. These results consistently demonstrate that hydrogenation at C1 is preferred across all three transition-metal surfaces. All the corresponding IS, TS, and FS structures on the three metals are shown in Fig. 3.

The second hydrogenation stage proceeds from the Furan-1H* intermediate and involves exploring potential hydrogen additions at the remaining ring carbons (C2, C3, and C4). On Pd (111), the most favorable pathway corresponds to hydrogen addition at C2, with an activation barrier of 0.98 eV and a reaction energy of 0.40 eV. Alternative routes like hydrogenation at C3 (1.35 eV barrier) and at C4 (1.15 eV barrier) are both kinetically less favorable. Thus, on Pd (111), the pathway leading to hydrogenation at C2 is preferred, yielding the Furan-2H* intermediate. All competing barriers and reaction energies are summarized in Table 1.

On Pt (111), however, the energetics differ. Following the first hydrogenation at the C1, the second hydrogenation is also kinetically favored at the symmetry-related α -site, C4. This pathway exhibits a barrier of only 0.70 eV and a slightly endergonic reaction energy of 0.03 eV. In comparison, hydrogenation at C2 and C3 requires higher barriers of 1.06 eV and 1.05 eV, respectively, with reaction energies of 0.12 eV and 0.20 eV. These results indicate that Pt (111) favors consecutive hydrogenation of α -carbons. A similar trend is observed on Ni (111). After the initial hydrogenation at C1, the kinetically most favorable second hydrogenation also occurs at C4, with a barrier of 0.71 eV. The step is moderately endothermic, with a reaction energy of 0.57 eV.

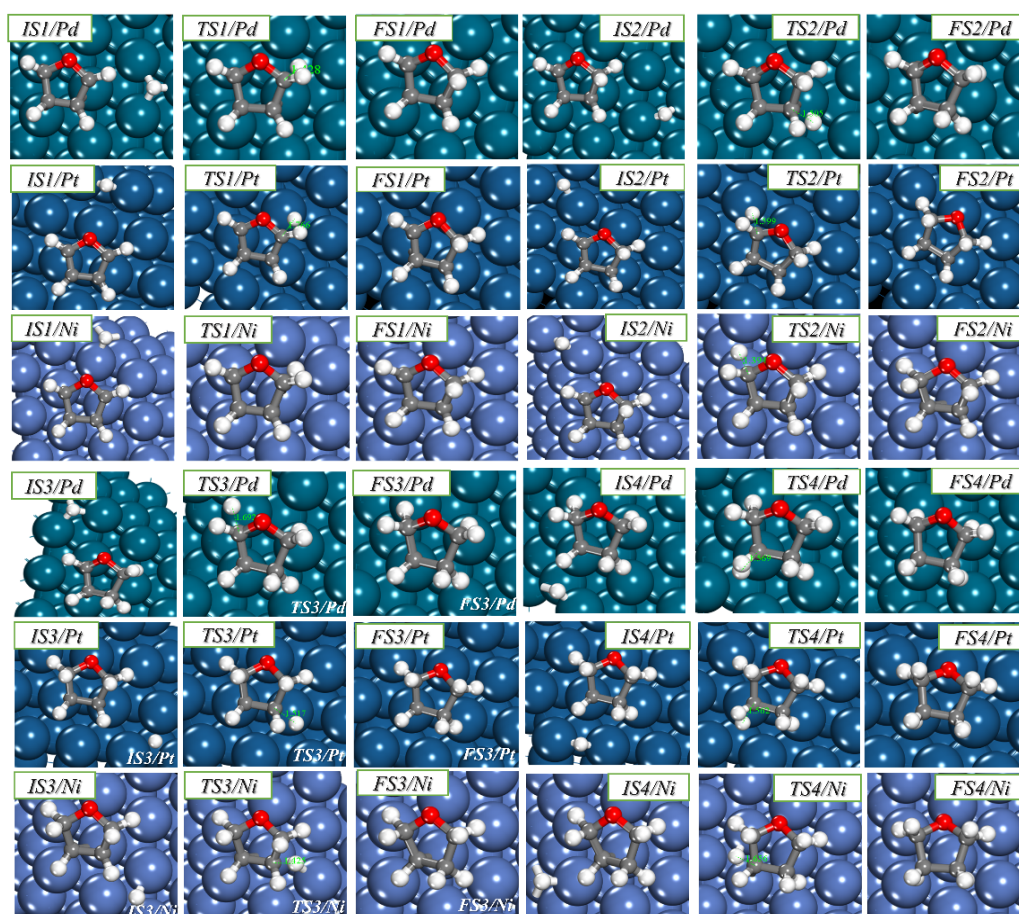


Fig. 3. The Initial states (IS1–IS4), Transition states (TS1–TS4), and Final states (FS1–FS4) for furan hydrogenation to THF on Pd (111), Ni (111), and Pt (111) surfaces.

Table 1. Activation energies (eV) and reaction energies (eV) for the competitive hydrogenation pathways from furan to tetrahydrofuran over three metal surfaces

Steps	Hydrogen Addition Site	Pd (111)		Pt (111)		Ni (111)	
		E_a (eV)	ΔE_R (eV)	E_a (eV)	ΔE_R (eV)	E_a (eV)	ΔE_R (eV)
First step	C1	0.94	0.49	0.54	-0.26	0.86	0.47
	C2	1.23	0.60	0.63	-0.14	1.52	0.67
Second step	C2	0.98	0.40	1.06	0.12	1.50	0.27
	C3	1.35	0.80	1.05	0.2	1.21	0.80
	C4	1.15	0.57	0.70	0.03	0.71	0.57
Third step	C2	-	-	1.02	0.46	0.61	0.55
	C3	1.16	0.43	1.0	0.47	1.21	0.46
	C4	1.10	0.74	-	-	-	-
Fourth step	C3	1.04	0.07	1.00	0.01	0.89	-0.3

Note: For each hydrogen-addition step, the site with the lowest activation barrier is highlighted in blue (e.g., C1 in Step 1, C2 in Step 2 for Pd)

To understand these mechanistic differences, Bader charge analysis was carried out for the second hydrogenation step (Furan-1H* + H → Furan-2H*) on three surfaces. The charge variations ($\Delta q = q_{FS} - q_{IS}$, where q_{IS} and q_{FS} correspond to the Bader charges of the atom in the initial and final states, respectively) quantify both the direction and magnitude of charge transfer during hydrogen addition. On Pt, the hydrogenation at the C4 site shows the most balanced and favorable charge transfer. Here, the Furan-1H* fragment loses approximately +0.25 e, while the Pt surface and the incoming H atom each gain about -0.12 e. This indicates that electrons transfer from the furan ring toward both the Pt surface and the hydrogen atom. Such cooperative charge transfer (furan → H and furan → Pt) stabilizes C-H bond formation, leading to a lower reaction barrier on Pt. In comparison, hydrogenation at C2 primarily involves charge transfer from the Pt surface to the incoming H atom, while in the C3 hydrogenation pathway, both furan and Pt donate smaller amounts of charge. Therefore, hydrogenation at C4 is the most favorable on Pt (111) due to strong and well-balanced charge redistribution. A similar trend is observed for Ni. In the C4 hydrogenation step, both the Ni surface and the Furan-1H* molecule lose nearly equal charge (~ +0.14 e each), while the hydrogen atom gains around -0.29 e. This indicates that the electrons transfer from both Ni and the adsorbate toward H, forming a hydride-like H that stabilizes the new C-H bond. In contrast, C2 hydrogenation draws charge primarily from Ni, and the C3 pathway involves smaller and less cooperative charge donation from both Ni and furan. Thus, as with Pt, hydrogenation at C4 is energetically preferred on Ni (111) owing to its more cooperative and well-distributed electron transfer. For Pd, however, the second hydrogenation step shows a different trend. In the hydrogenation at C2, both Pd and Furan-1H* lose electrons (+0.054 e, +0.141 e), while the H atom gains a significant amount of charge (-0.195 e). This indicates that electrons transfer from both the Pd surface and the adsorbate toward H, forming a hydride-like H and stabilizing the newly forming C-H bond. In the other hydrogenation pathways, either Pd is the primary electron donor or the overall charge transfer is smaller and less coordinated. Therefore, unlike Pt and Ni, the C2 hydrogenation route is preferred on Pd (111) due to its lower kinetic barrier and more favorable charge redistribution.

For the third hydrogenation, on Pd (111), with C1 and C2 already saturated, the next hydrogen addition was examined

at C3 and C4. Hydrogenation at C4 emerged as the preferred pathway, with an activation barrier of 1.10 eV and a reaction energy of 0.74 eV, compared to a slightly higher barrier of 1.16 eV ($\Delta E_R = 0.43$ eV) at C3. This step constitutes the Rate-Determining Step (RDS) of the overall hydrogenation sequence on Pd, yielding the Furan-3H* intermediate. On Pt (111), since C1 and C4 were already hydrogenated, possible H additions at C2 and C3 were analyzed. The barriers were nearly identical, 1.02 eV ($\Delta E_R = 0.46$ eV) for C2 and 1.03 eV ($\Delta E_R = 0.47$ eV) for C3, making the two sites kinetically competitive. Nonetheless, hydrogenation at C2 is slightly more favorable and constitutes the RDS on Pt (111). On Ni (111), hydrogenation at C2 was strongly favored with a barrier of 0.61 eV and reaction energy change of 0.55 eV, whereas C3 hydrogenation required a significantly larger barrier of 1.21 eV, making it non-competitive. This mechanistic divergence highlights that, unlike Pt (111), Ni (111) shows a clear preference for C2 hydrogenation without significant competition from C3.

The fourth and final hydrogenation step converts Furan-3H* to Furan-4H* (THF) by saturating the remaining unsaturated carbon (C3) on the intermediate. On Pd (111), hydrogenation at C3 exhibits an activation barrier of 1.04 eV and an almost thermoneutral reaction energy of 0.07 eV. On Pt (111), the C3 hydrogenation requires a comparable barrier of 1.00 eV with a nearly zero reaction energy change of 0.01 eV. For Ni (111), this step is slightly exothermic ($\Delta E_R = -0.30$ eV) with an activation barrier of 0.89 eV, making it the RDS on Ni (111). The fully hydrogenated THF molecule binds weakly to all three metal surfaces, consistent with physisorption, which facilitates easy desorption under reaction conditions. Considering the overall hydrogenation sequence, the most favorable pathway on Pd (111) is C1 → C2 → C4 → C3. In contrast, on Pt (111) and Ni (111), the preferred sequence is C1 → C4 → C2 → C3. Fig. 4 presents the corresponding potential energy profiles for all surfaces, highlighting the key intermediates.

The RDS for Pd (111) is the third hydrogenation step at C4, with an activation barrier of 1.10 eV and a reaction energy of 0.74 eV. On Pt (111), the RDS is the third hydrogenation at C2, with an activation barrier of 1.02 eV and a reaction energy of 0.46 eV. For Ni (111), the fourth hydrogenation step at C3 is rate-limiting, with an activation barrier of 0.89 eV and a reaction energy of -0.30 eV. From the DFT results, Ni (111) appears to be the most active surface for THF formation, exhibiting the lowest activation barrier for

the rate-determining step. However, Sithisa *et al.* [4] reported that THF was not detected over Ni-based catalysts, likely due to rapid ring opening to products such as butanal, butanol, and butane. In our study, these ring-opening pathways were not considered, which may explain the discrepancy between DFT predictions and experimental observations. In contrast, Pd-based catalysts exhibit superior performance, showing higher selectivity toward THF under relatively mild reaction conditions [22, 23]. Our results elucidate the specific pathways on Pt and Pd surfaces. Incorporating temperature corrections and performing microkinetic modelling would yield a more realistic representation of experimental behavior.

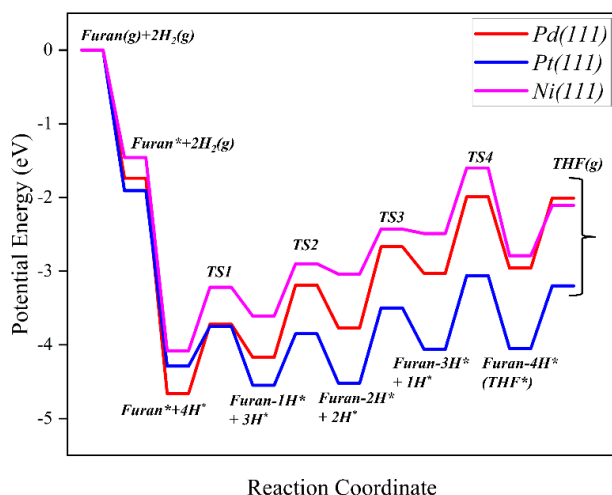


Fig. 4. PES for the complete hydrogenation of Furan to THF on three metal surfaces. The process involves four consecutive hydrogenation steps, starting from adsorbed furan and hydrogen atoms, and ending with THF formation and desorption.

This study provides an atomistic insight into the entire hydrogenation process from furan to THF on three metal surfaces. These results bridge the gap between DFT predictions and experimentally observed trends, enabling the rational development of future bimetallic or supported catalysts with Ni-like activity and Pd/Pt-like selectivity. In addition, the energetic data from this research can be used as the basis of subsequent microkinetic and solvent-based simulations of biomass hydrogenation.

V. CONCLUSION

In this study, we performed a comprehensive DFT study to evaluate the adsorption behavior and hydrogenation pathways of Furan to Tetrahydrofuran (THF) on Pd (111), Pt (111), and Ni (111) surfaces. Furan preferentially adsorbs in a flat configuration at the fcc site with binding energies of -1.74 eV, -1.91 eV, and -1.46 eV on Pd, Pt, and Ni, respectively, while THF binds weakly (-0.95 eV, -0.85 eV, -0.68 eV), indicating facile desorption. The successive hydrogenation of furan proceeds through distinct pathways depending on the metal: the most favorable pathway on Pd (111) is $C1 \rightarrow C2 \rightarrow C4 \rightarrow C3$, whereas Pt (111) and Ni (111) follow the $C1 \rightarrow C4 \rightarrow C2 \rightarrow C3$ pathway. To explain these mechanistic discrepancies, we conducted a comprehensive Bader charge analysis for the second hydrogenation step. This investigation revealed that the distribution of electron density between reacting carbon and hydrogen atoms varies

between metals, which explains why preferred hydrogenation sequences and rate-determining steps differ. The rate-determining steps differ across the metals, with the third hydrogenation at C4 (~ 1.10 eV) limiting the overall reaction on Pd (111), the third hydrogenation at C2 (~ 1.02 eV) as the RDS on Pt (111), and the final hydrogenation at C3 (~ 0.89 eV) being rate-limiting on Ni (111). Although Ni (111) appears highly active, experimental results show that it tends to promote ring-opening or over-hydrogenation rather than THF formation. Nevertheless, the present work clarifies the complete hydrogenation pathways on these metals.

CONFLICT OF INTEREST

The authors declare no competing financial interest.

AUTHOR CONTRIBUTIONS

Saikat Saha: Conceptualization, methodology, investigation, formal analysis, data curation, software, validation, visualization, writing—original draft, writing—review & editing. Sanjay M. Mahajani: Supervision, project administration, funding acquisition, writing—review & editing. Akkihebbal K. Suresh: Supervision, project administration, funding acquisition, writing—review & editing. Ojus Mohan: Conceptualization, methodology, validation, supervision, writing—review & editing, visualization. All authors had approved the final version.

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