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Descriptor-Based Screening of Nanocatalysts for CO_2 Conversion: A Computational Data-Driven Study

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ABSTRACT: CO_2 conversion is a central strategy for closing the carbon cycle and enabling sustainable energy and chemical production through catalytic pathways. In this work, a descriptor-based, data-driven computational framework is employed to screen nanocatalysts for CO_2 conversion using density functional theory data reported in the literature. Key adsorption and electronic descriptors, including CO_2* and $CO*$ binding energies, are analyzed to establish structure-activity relationships governing catalytic performance. Correlation and volcano-type analyses reveal that moderate adsorption strengths are essential for balancing CO_2 activation and product desorption, while excessively strong binding leads to surface poisoning and reduced activity. The results demonstrate that descriptor-guided screening can effectively rank catalyst candidates and provide rational design rules, without relying on new, computationally intensive simulations. This framework offers a computationally efficient pathway for accelerating nanocatalyst discovery for CO_2 conversion.

1. INTRODUCTION

The continuous rise in atmospheric carbon dioxide (CO_2) concentration has intensified global efforts toward sustainable energy and chemical production. Catalytic CO_2 conversion is widely recognized as a key strategy for eliminating carbon by transforming captured CO_2 into value added fuels and chemicals using renewable energy sources [1]. However, the rational design of efficient and selective catalysts remains challenging due to the thermodynamic stability of CO_2 and the complexity of reaction intermediates involved. Nanostructured catalysts, including metal nanoparticles and single-atom catalysts, have emerged as promising candidates for CO_2 conversion owing to their high surface area and tunable electronic properties [2]. Density functional theory (DFT) has played a central role in understanding catalytic mechanisms and guiding the catalyst development [4]. Nevertheless, comprehensive DFT-based reaction pathway and microkinetic studies are computationally demanding, motivating the adoption of descriptor-based approaches that rely on a reduced set of key energetic and electronic parameters to capture catalytic trends [5]. Descriptor-guided screening exploits fundamental relationships between adsorption energies and catalytic activity, enabling efficient catalyst ranking through volcano-type relationships [6]. More recently, data-driven screening strategies and single-atom catalyst design have further accelerated catalyst discovery for CO_2 conversion [7–9]. Such data-driven frameworks enable rapid catalyst down-selection while avoiding the high computational cost associated with reaction pathway calculations, making them attractive for early-stage catalyst discovery [8]. In this study, a literature-based, descriptor-driven computational framework is employed to identify structure activity trends and establish some designed rules for nanocatalysts for CO_2 conversion.

2. MATERIALS AND METHODS

This study presents a literature-based, data-driven computational analysis of nanocatalysts for CO_2 conversion. Peer-reviewed publications reporting density functional theory (DFT) investigations of nanostructured catalysts were systematically collected from major scientific databases, including Web of Science, Scopus, ScienceDirect, ACS Publications, SpringerLink, and MDPI. Only studies employing well-established DFT methodologies, as modeled in Figure 1 and clearly defined adsorption configurations were considered to ensure data consistency and reliability. The collected data were standardized and analyzed using Python-based data processing and visualization tools within a Jupyter Notebook environment. Descriptor correlations, volcano-type relationships, and catalyst ranking analyses were employed to identify structure-activity trends governing CO_2 conversion performance. Molecular and schematic visualizations were generated using Avogadro software to illustrate representative adsorption configurations and catalyst models. All data analyzed in this work were obtained from previously published sources and are appropriately cited.

2.1. Limitations and Consistency of Literature-Derived DFT Data

This study relies on adsorption energies and activity trends reported in previously published density functional theory (DFT) investigations. It is well known that DFT results obtained from different studies may vary due to differences in exchange-

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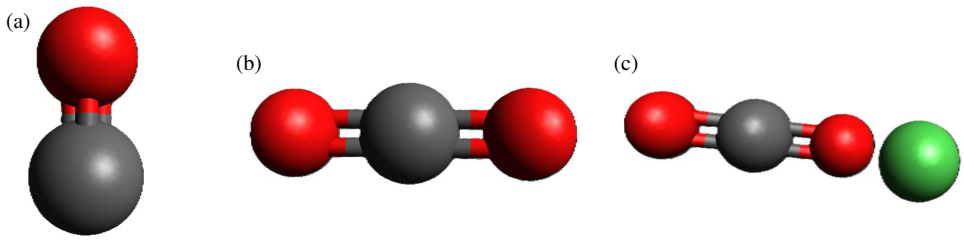

FIGURE 1. (a) Ball-and-stick representation of CO, (b) linear CO_2 molecule, and (c) schematic illustration of CO_2 adsorption on a Ni single-atom nanocatalyst. The structures are shown for visualization purposes and do not represent optimized geometries.

correlation functionals, plane-wave cut-off energies, slab thicknesses, surface facets, and k-point sampling. As a result, absolute adsorption energies reported across the literature may not be directly comparable on a quantitative basis. In this work, the limitations are addressed by focusing on relative trends and qualitative correlations rather than absolute energetic values. Only studies employing clearly defined adsorption configurations and comparable surface models were considered, and the descriptor analysis is interpreted as a trend-based screening rather than a predictive kinetic model. Consequently, the proposed framework is intended for relative catalyst ranking and early-stage down selection, rather than quantitative prediction of catalytic rates or selectivities.

3. RESULTS AND DISCUSSION

3.1. Descriptor Correlation Analysis

A positive correlation is observed between the CO_2* and $CO*$ adsorption energies, indicating that catalysts exhibiting strong CO_2 binding tend to also stabilize CO intermediates. Quantitatively, the correlation between CO_2* and $CO*$ adsorption energies yields a Pearson correlation coefficient of $r \approx 0.75$–0.80, indicating strong coupling between the adsorption behaviors of these carbon-containing intermediates across the examined catalyst systems. Figure 2 presents the correlation matrix between key adsorption descriptors and normalized catalytic activity for the selected nanocatalysts. This behavior is consistent with

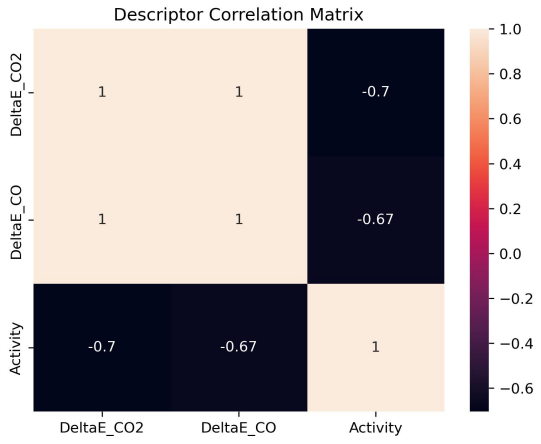

FIGURE 2. Correlation matrix showing the relationships among CO_2* adsorption energy, $CO*$ adsorption energy, and normalized catalytic activity for the selected nanocatalysts.

the electronic structure similarity governing the adsorption of carbon-containing species on transition metal sites [4, 5].

3.2. Rationale for Descriptor Selection

The choice of CO_2* and $CO*$ adsorption energies as primary descriptors is motivated by their mechanistic relevance in CO_2 conversion pathways. CO_2* adsorption energy is commonly regarded as a proxy for CO2 activation, reflecting the ability of a catalyst surface to stabilize and bend the linear CO_2 molecule during the initial activation step. In contrast, $CO*$ adsorption energy is closely associated with subsequent reaction progression and product desorption, as excessively strong CO binding can lead to surface site blocking and catalyst poisoning. Together, these two descriptors capture complementary aspects of the catalytic process, balancing reactant activation and intermediate removal. Other potentially relevant descriptors, such as $O*$, $OH*$, or $CHO*$ adsorption energies and electronic structure parameters (e.g., d-band center or charge transfer), were considered; however, their inconsistent reporting across the literature precluded statistically meaningful aggregation within a unified dataset. Therefore, CO_2* and $CO*$ adsorption energies were selected as transferable and widely reported descriptors suitable for literature-based screening. Recent comprehensive reviews have further validated the use of adsorption-energy descriptors for capturing activity and selectivity trends in CO_2 conversion, while emphasizing their role as physically interpretable screening metrics rather than complete kinetic models [10].

In contrast, a clear negative correlation is observed between adsorption strength and catalytic activity. Both CO_2* and $CO*$ adsorption energies show moderate negative correlations with activity, suggesting that excessively strong binding can hinder catalytic performance by limiting product desorption or blocking active sites. Such trends are well aligned with the Sabatier principle, which states that optimal catalytic activity is achieved at intermediate adsorption strengths rather than at extremes of strong or weak binding [5]. These results demonstrate that descriptor-based analysis can effectively capture fundamental structure-activity relationships using literature-derived data.

3.3. Volcano-Type Activity Relationship

The relationship between $CO*$ adsorption energy and normalized catalytic activity is further illustrated in Figure 3 through a volcano-type plot. Despite the limited size of the dataset, a clear trend is evident, with catalysts exhibiting moderate CO_2 adsorption energies achieving higher activity compared to those

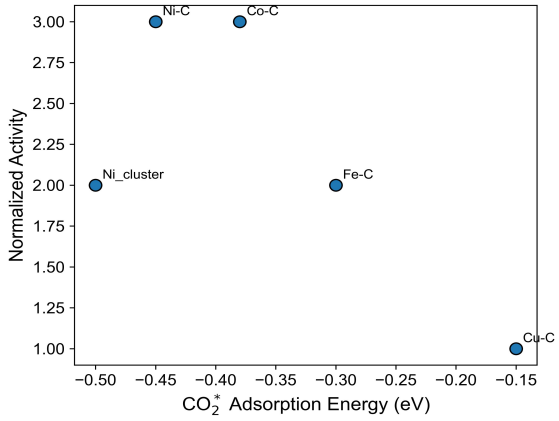

FIGURE 3. Volcano-type relationship between CO_2* adsorption energy and normalized catalytic activity.

with either very weak or very strong binding. Ni- and Co-based single-atom catalysts occupy favorable regions of the activity landscape, while Cu-based systems with weak adsorption and Ni cluster models with stronger binding display reduced performance.

This volcano-type behavior reflects the balance required between CO_2 activation and subsequent reaction or desorption steps, a characteristic feature of heterogeneous catalysis [6]. Catalysts with overly strong adsorption may suffer from surface poisoning by reaction intermediates, whereas weakly binding catalysts may fail to sufficiently activate the CO_2 molecule. The observed trends are consistent with previous theoretical studies, highlighting adsorption energy descriptors as reliable predictors of catalytic performance in CO_2 conversion reactions [3].

3.4. Descriptor-Based Catalyst Screening

Based on the descriptor analysis, a simple ranking of catalyst candidates was established using CO_2 adsorption energy as the primary screening parameter (Table 1). Catalysts with adsorption energies near the optimal intermediate range were ranked highest, reinforcing the utility of descriptor-guided screening for narrowing down promising catalyst candidates. Importantly, this approach enables rapid evaluation of diverse catalyst systems without the need for new computationally intensive simulations.

TABLE 1. Descriptor-based screening of selected nanocatalysts for CO_2 conversion using literature-derived adsorption energies.

Catalyst	Type	ΔE_{CO_2} (eV)	ΔE_{CO} (eV)	Activity
Ni-C	SAC	−0.45	−0.62	High
Fe-C	SAC	−0.30	−0.48	Medium
Co-C	SAC	−0.38	−0.55	High
Cu-C	SAC	−0.15	−0.30	Low
Ni cluster	Cluster	−0.50	−0.70	Medium

Overall, the results demonstrate that literature-based, data-driven descriptor analysis can provide meaningful insights into catalyst performance trends and support rational nanocatalyst design. By leveraging established DFT data and fundamental catalytic principles, this frame-work offers an efficient pathway for accelerating catalyst discovery for CO_2 conversion while minimizing computational cost.

4. EXTENSION OF DESCRIPTOR-BASED ANALYSIS TO MULTIMETAL AND HIGH-ENTROPY ALLOY CATALYSTS

4.1. Scope of Descriptor Application to Multimetal and HEA Catalysts

When extending adsorption-based descriptors to multimetallic and high-entropy alloy (HEA) catalysts, it is important to recognize that these chemically complex systems exhibit local atomic heterogeneity, electronic reconstruction, and synergistic effects that are not explicitly resolved by a single averaged descriptor. In this work, CO_2 and CO adsorption energies are interpreted as an effective surface-averaged property that captures dominant adsorption trends rather than site-specific interactions. As such, the descriptor-based analysis does not aim to resolve local active motifs or elemental segregation effects, but instead provides a first-order screening metric for identifying promising compositional regions within a vast multimetal design space. The observed volcano-type behavior across both monometallic and multimetal systems therefore supports the qualitative transferability of adsorption-energy descriptors at the screening level, while detailed mechanistic understanding of HEA catalysts requires subsequent targeted DFT calculations or experimental validation.

4.2. Extension Study

To evaluate the transferability of adsorption-based descriptors beyond monometallic and single-atom catalysts, the descriptor framework was further extended to representative multimetal and high-entropy alloy (HEA) catalyst systems using literature-reported CO adsorption energies. Specifically, multimetal surfaces and equiatomic HEAs composed of transition metals commonly employed in CO_2 conversion catalysis — including Ni, Co, Fe, Cu, and Pd were considered. These elements are frequently incorporated into HEAs to tune adsorption strength through electronic and ensemble effects, making them suitable model systems for descriptor-based trend analysis. CO adsorption was selected as the primary descriptor for this extension due to its well-established role as a key reaction intermediate and potential site-blocking species in CO_2 conversion pathways. Moreover, CO adsorption energies are more consistently reported for multimetal and alloy surfaces than CO_2 adsorption energies, enabling a coherent comparison across chemically complex catalyst systems. Previous theoretical studies have demonstrated that CO adsorption strength correlates strongly with catalytic activity and selectivity through its influence on intermediate stabilization and surface poisoning effects [4]. Scaling relationships linking CO adsorption to other carbon-containing intermediates further support its use as a transferable descriptor across diverse catalyst classes [5]. Fig-

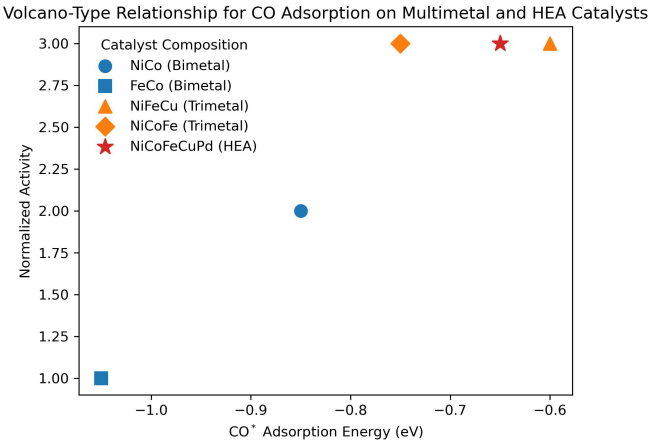

FIGURE 4. Volcano-type relationship between CO adsorption energy and normalized catalytic activity for representative multimetal and high-entropy alloy catalysts.

ure 4 presents a volcano-type relationship between CO adsorption energy and normalized catalytic activity for selected multimetal and HEA catalysts, including NiCo, FeCo, NiFeCu, and the equiatomic NiCoFeCuPd HEA. A clear qualitative trend is observed, with optimal activity located at intermediate CO adsorption strengths. Catalysts exhibiting excessively strong CO binding are expected to experience surface site blocking, while weakly binding systems may be insufficient to stabilize key reaction intermediates. The persistence of this volcano-type behavior across both simple and chemically complex catalyst systems highlights the robustness and transferability of adsorption-based descriptors.

The derived CO adsorption energies for representative multimetal and high-entropy alloy catalysts are summarized in Table 2. This extension demonstrates that the descriptor-based framework employed in this study is not restricted to a specific catalyst class, but can be readily applied to multimetal and HEA systems. This finding reinforces the suitability of lightweight, adsorption energy driven screening strategies for early-stage catalyst discovery across a broad compositional design space, including chemically complex alloys.

TABLE 2. Literature-derived CO adsorption energies for representative multimetal and high-entropy alloy catalysts.

Catalyst	Type	ΔE_{CO} (eV)	Activity
NiCo	Bimetal	−0.85	Medium
FeCo	Bimetal	−1.05	Low
NiFeCu	Trimetal	−0.60	High
NiCu	Bimetal	−0.35	Low
NiCoFe	Trimetal	−0.75	High
NiCoFeCuPd	HEA	−0.65	High

While recent advances in catalyst discovery increasingly rely on large-scale high-throughput computations and machine-learning-based screening, such approaches often require substantial computational resources, complex model training, and limited interpretability of the resulting predictions. In contrast, the present work focuses on a lightweight, descriptor-based screening strategy that directly reuses high-quality density functional theory data reported in the literature to extract physically meaningful structure-activity trends.

Rather than competing with data-intensive machine learning frameworks in terms of dataset size, the proposed approach emphasizes transparency, interpretability, and computational accessibility. By combining adsorption-energy descriptors with straightforward statistical and volcano-type analyses, the framework enables rapid catalyst down-selection and hypothesis generation at negligible computational cost. Comprehensive recent reviews further emphasize that adsorption-energy descriptors remain valuable for narrowing the HEA design space, provided their limitations are explicitly acknowledged and complemented by targeted high-fidelity modeling or experimental validation [11].

5. CONCLUSIONS

In this study, a descriptor-based, data-driven computational framework was employed to screen nanocatalysts for CO_2 conversion using literature-derived density functional theory data. By analyzing key adsorption descriptors, including CO_2* and $CO*$ adsorption energies, fundamental structure-activity relationships governing catalytic performance were identified without performing new computationally intensive simulations. Correlation analysis revealed a strong coupling between CO_2 and CO adsorption energies, indicating similar adsorption trends across transition-metal-based catalyst systems. A negative correlation between adsorption strength and catalytic activity highlights the importance of moderate binding energies for achieving optimal performance, consistent with the Sabatier principle. Volcano-type analysis further demonstrated that catalysts with intermediate CO_2 adsorption strengths occupy favorable regions of the activity landscape, while excessively strong or weak adsorption leads to reduced activity. The descriptor-guided screening results identified Ni- and Co-based single-atom catalysts as promising candidates for CO_2 conversion, emphasizing the effectiveness of adsorption energy descriptors for rapid catalyst evaluation. Overall, this work demonstrates that literature-based, data-driven descriptor analysis provides a practical and computationally efficient pathway for rational nanocatalyst design. The presented framework can be readily extended to other catalytic reactions and material systems, supporting the accelerated discovery of efficient catalysts for sustainable CO_2 conversion technologies.

Scope and Predictive Boundaries of the Framework

The descriptor-based framework presented in this study is intended as a lightweight, computationally efficient screening tool rather than a comprehensive predictive model. It is effective for identifying relative activity trends, ranking catalyst candidates, and generating physically grounded hypotheses for further investigation. The approach does not explicitly capture reaction kinetics, coverage effects, surface reconstruction, or reaction-condition-dependent phenomena, nor does it replace detailed reaction pathway analysis or microkinetic modeling. So, the framework is best applied at the early stages of cata-

lyst discovery to guide the selection of promising systems for subsequent high-fidelity DFT calculations or experimental validation.

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