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Single-Atom Catalysts Based on Two-Dimensional Transition Metal Carbides for Efficient Carbon Dioxide Reduction

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Abstract: The electrochemical reduction of carbon dioxide (CO_2RR) into value-added products is a promising route toward carbon neutrality, yet its efficiency is often limited by the weak activity and instability of conventional catalysts. Single-atom catalysts (SACs) anchored on two-dimensional transition metal carbides (MXenes) offer a tunable platform with high atomic utilization and strong metal-support interactions. However, the fundamental understanding of how coordination geometry and electronic coupling jointly regulate CO_2 activation remains insufficient. This study integrates density functional theory (DFT) calculations with experimental electrochemical characterization to investigate MXene-supported SACs. The $Fe_1/Ti_3C_2O_2$ system exhibits a pseudo-square-planar coordination environment with strong Fe-O bonding, leading to an optimized d-band alignment and enhanced σ-back-donation to $CO_2\pi^*$ orbitals. The calculated free-energy barrier for COOH formation is only 0.41 eV, resulting in high Faradaic efficiency (91.2%) and a partial current density of 34.8 $mA\cdot cm^{-2}$. These findings reveal that ligand field stabilization and interfacial charge transfer are key to achieving efficient CO_2 reduction. The proposed coordination-electronic coupling framework provides actionable guidelines for the rational design of high-performance catalytic materials in sustainable energy conversion.

Keywords: MXene; single-atom catalyst; coordination chemistry; CO_2 reduction; electronic coupling; surface catalysis

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1. Introduction

The anthropogenic emission of carbon dioxide (CO_2) has intensified the global energy and environmental crisis, urging the development of sustainable technologies that can close the carbon cycle [1]. Among various approaches, the electrochemical CO_2 reduction reaction (CO_2RR) has emerged as a promising route for converting CO_2 into value-added chemicals and fuels under mild conditions [2]. The design of highly efficient, selective, and durable electrocatalysts lies at the heart of achieving practical CO_2 conversion. In this context, understanding the interplay between atomic coordination, electronic structure, and surface reaction pathways has become a central challenge in materials chemistry and catalysis science [3].

Conventional metallic or oxide catalysts often suffer from low atom utilization, broad active-site distributions, and competing side reactions such as hydrogen evolution. Single-atom catalysts (SACs), featuring isolated metal atoms anchored on well-defined supports, provide a powerful strategy to overcome these limitations [4]. Their atomically dispersed nature maximizes the exposure of active sites and enables precise tuning of the coordination environment. However, the catalytic performance of SACs is strongly governed by the interaction between the single metal atoms and their substrate, where electronic coupling, charge transfer, and local bonding geometry jointly determine the reaction energetics [5]. Achieving both atomic stability and optimized adsorption behavior therefore requires a rationally designed support that can simultaneously stabilize single atoms and modulate their electronic states.

Two-dimensional transition metal carbides, commonly known as MXenes, have recently emerged as a new class of catalyst supports with unique structural and chemical features [6]. Their metallic conductivity, high surface area, and adjustable surface terminations (e.g., -O, -F, -OH) offer exceptional tunability of electronic properties. Moreover, the strong metal-support interactions intrinsic to carbides can effectively prevent metal atom migration and aggregation. These attributes make MXenes particularly attractive for hosting single-atom sites. Nevertheless, despite extensive experimental efforts, the fundamental understanding of how MXene surface chemistry governs the coordination environment, electronic redistribution, and catalytic activity of single atoms remains insufficient. In particular, the correlation between surface terminations, metal d-band modulation, and CO_2 intermediate binding strength has not been comprehensively clarified.

This study aims to establish a theoretical-experimental framework that elucidates the coordination-electronic coupling mechanisms in MXene-supported single-atom catalysts for CO_2 reduction. By integrating density functional theory (DFT) calculations with electrochemical performance evaluation, the work systematically explores how surface terminations and interfacial bonding influence the adsorption and activation of CO_2 molecules. The study further compares different transition-metal centers to identify optimal coordination configurations that minimize the energy barrier of the rate-determining step. Through a combination of surface characterization and electronic structure analysis, the research provides direct evidence linking coordination geometry with catalytic kinetics.

The novelty of this work lies in its interdisciplinary approach bridging coordination chemistry, surface catalysis, and materials design. Rather than focusing solely on performance optimization, the research emphasizes mechanistic understanding at the atomic scale, providing a unified view of how local chemical environments drive macroscopic catalytic behavior. The findings not only enrich the theoretical foundation of single-atom catalysis but also offer practical guidance for designing next-generation electrocatalysts with high activity and selectivity. By unveiling the structure-function relationships governing MXene-anchored single-atom catalysts, this study contributes to advancing carbon-neutral energy conversion technologies and deepening the fundamental understanding of catalytic materials chemistry.

2. Literature Review

The development of SACs has revolutionized the field of heterogeneous catalysis by bridging the gap between homogeneous and heterogeneous systems [7]. Their atomically dispersed active sites allow precise control of coordination geometry, enabling a direct relationship between local electronic structure and catalytic performance [8]. Previous studies have demonstrated that SACs exhibit exceptional atom utilization efficiency and unique selectivity for multi-electron reactions such as CO_2 reduction, nitrogen fixation, and oxygen evolution. The well-defined coordination environments of SACs facilitate mechanistic understanding through both theoretical modeling and spectroscopic characterization, making them ideal systems for fundamental catalytic research [9].

Despite these advantages, conventional SACs supported on carbon, oxides, or nitrides face persistent challenges. Carbon-based supports often lack sufficient metal-support interaction, leading to atom migration and aggregation during electrochemical operation [10]. Oxide or nitride supports can provide stronger binding but frequently suffer from low electrical conductivity, which limits charge transfer during catalytic reactions. Furthermore, the chemical inertness of these substrates restricts their ability to modulate the electronic structure of anchored metal atoms. Consequently, the delicate balance between stability and activity remains difficult to achieve, and the mechanistic understanding of support-metal synergy is still incomplete [11].

Recent progress in two-dimensional (2D) materials has introduced new possibilities for SAC design. Graphene and transition-metal dichalcogenides (TMDs) have been investigated as conductive supports that offer abundant surface sites [12]. However, the lack of strong chemical bonding between single atoms and these inert surfaces often results in limited long-term stability. Compared with these materials, 2D transition metal carbides, commonly referred to as MXenes, have emerged as highly promising supports due to their metallic conductivity, hydrophilicity, and tunable surface terminations [13]. Their unique combination of transition-metal layers and surface functional groups allows precise engineering of electronic and structural properties, making them ideal hosts for stabilizing single metal atoms.

Nevertheless, the current understanding of MXene-based SACs remains fragmented. While experimental work has confirmed enhanced activity in some MXene-supported systems, the underlying coordination mechanisms and electronic coupling processes are still not fully clarified [14]. The role of surface terminations (such as -O and -F) in defining the charge redistribution between the single metal center and the carbide substrate has not been systematically quantified. Similarly, the relationship between the local coordination symmetry and the binding strength of CO_2 intermediates is still under debate. Without a comprehensive theoretical framework, it is difficult to rationally predict or tune the catalytic behavior of these hybrid systems.

Comparative analyses between MXene-supported SACs and other 2D materials suggest that the superior catalytic performance of MXenes arises from the strong d-d orbital overlap between transition-metal atoms and surface terminations, which enhances the adsorption of key intermediates and reduces energy barriers for CO_2 activation [15]. However, most existing studies focus primarily on empirical performance metrics, with limited integration of electronic-structure analysis or in-situ characterization. This lack of mechanistic insight prevents the establishment of universal design principles for MXene-based catalysts.

In response to these gaps, the present study develops a unified theoretical-experimental framework to elucidate how the coordination environment and electronic modulation of single-atom sites on MXene surfaces dictate CO_2 reduction activity. By systematically correlating DFT predictions with experimental electrochemical results, this research aims to reveal the governing principles of charge redistribution and intermediate binding on MXene-supported SACs. The study thus extends the frontiers of materials chemistry and surface catalysis, contributing to the rational design of efficient, stable, and tunable catalysts for sustainable energy conversion.

3. Theoretical Framework and Methodology

3.1. Theoretical Framework

The catalytic reduction of carbon dioxide on single-atom catalysts (SACs) supported by two-dimensional transition metal carbides (MXenes) can be understood through the combined perspectives of coordination chemistry and surface catalytic thermodynamics. In SAC systems, the activity and selectivity of a reaction are primarily governed by the coordination environment of the metal center, the charge transfer at the metal-support interface, and the adsorption-desorption dynamics of reaction intermediates.

The local electronic environment of the single metal atom is dominated by its coordination number and ligand field strength. The crystal-field splitting energy, which determines the occupancy of d-orbitals, can be expressed as:

$$\Delta_{cf} = k_1 \frac{Z_{eff}}{r^5} \tag{1}$$

where Z_{eff} is the effective nuclear charge, rrr is the average metal-ligand bond length, and k_1 is a proportionality constant dependent on coordination symmetry (octahedral or square-planar). In MXene-supported SACs, oxygen- and fluorine-terminated surfaces alter Z_{eff} by electron withdrawal, modifying the Δ_{cf} and thereby the d-band occupancy of the active center.

The d-band center model, widely used in surface catalysis, provides a quantitative correlation between the position of the metal's d-states and the adsorption strength of intermediates. The d-band center ε_d is defined as:

$$\varepsilon_d = \frac{\int E \cdot D_d(E)\, dE}{\int D_d(E)\, dE} \tag{2}$$

where $D_d(E)$ is the electronic density of d-states at energy E. A higher ε_d relative to the Fermi level enhances the overlap with adsorbate orbitals, strengthening chemisorption, whereas a deeper ε_d weakens adsorption. Achieving optimal catalytic performance thus requires balancing ε_d to follow the Sabatier principle, adsorption must be neither too strong nor too weak.

The surface reaction energetics for CO_2 reduction can be described by the free-energy change (ΔG) associated with key intermediates, particularly COOH and CO species:

$$\Delta G = \Delta E + \Delta ZPE - T\Delta S \tag{3}$$

where ΔE is the reaction energy from density functional theory (DFT) calculations, ΔZPE is the zero-point energy correction, T is the temperature, and ΔS is the entropy change between initial and final states. The thermodynamic descriptors ΔG_{COOH^*} and ΔG_{CO^*} are used to identify the rate-determining step (RDS). A smaller ΔG_{COOH^*} indicates easier CO_2 activation, while an appropriate ΔG_{CO^*} ensures facile CO desorption.

To connect coordination structure with reaction thermodynamics, a charge-transfer coefficient (η_{ct}) is defined as:

$$\eta_{ct} = \frac{Q_{M\to S}}{Q_{tot}} = \frac{\int [\rho_M(r) - \rho_S(r)]dV}{\int \rho_{tot}(r)\, dV} \tag{4}$$

where $Q_{M\to S}$ is the charge transferred from the metal center to the MXene substrate, $\rho_M(r)$ and $\rho_S(r)$ are the local charge densities of the metal and substrate, respectively, and Q_{tot} is the total electron density within the interface region. A moderate η_{ct} (typically 0.25-0.45) implies efficient electronic coupling conducive to stable adsorption of activated CO_2 species.

Finally, the catalytic activity can be expressed in terms of current density (j) under applied potential U using the ButlerVolmer formalism:

$$j = j_0\left[e^{-\alpha F(U-U_{eq})/RT} - e^{(1-\alpha)F(U-U_{eq})/RT}\right] \tag{5}$$

where j_0 is the exchange current density, α is the charge transfer coefficient, F is Faraday's constant, R is the gas constant, and U_{eq} is the equilibrium potential for CO_2 reduction. This equation establishes a bridge between computed free energies and measurable electrochemical performance.

3.2. Methodological Approach

This study integrates first-principles electronic structure simulation, spectroscopic validation, and electrochemical testing to elucidate the coordination-electronic interplay in MXene-supported SACs.

3.2.1. Computational Methods

Density functional theory (DFT) calculations are performed using a plane-wave basis with generalized gradient approximation (GGA) for exchange-correlation functionals. The projector augmented wave (PAW) method is employed to describe electron-ion interactions. A vacuum spacing of at least 15 Å is used to avoid interlayer interactions.

The binding energy of a single atom on MXene is computed as:

$$E_b = E_{SAC} - (E_{MXene} + E_{Metal}) \tag{6}$$

where E_{SAC} is the total energy of the optimized single-atom/MXene system, E_{MXene} is the pristine substrate energy, and E_{Metal} is the energy of an isolated metal atom. Negative E_b values indicate thermodynamic stability of the anchored atom. Charge density differences and Bader charge analyses are used to evaluate η_{ct} and to visualize electron redistribution.

3.2.2. Experimental Validation

MXene substrates (e.g., $Ti_3C_2T_x$) are synthesized through selective etching and delamination of MAX phases. Single atoms of transition metals (Fe, Ni, Co) are introduced via atomic layer deposition or wet-chemical impregnation, ensuring atomic dispersion.

Characterization techniques include:

X-ray photoelectron spectroscopy (XPS) to identify oxidation states and surface terminations.

Extended X-ray absorption fine structure (EXAFS) to determine coordination numbers and bond distances.

In-situ Fourier-transform infrared spectroscopy (FTIR) to monitor CO_2 intermediates under electrochemical bias.

3.2.3. Electrochemical Measurements

Catalytic performance is assessed using a gas-tight three-electrode system. Linear sweep voltammetry (LSV) and chronoamperometry are employed to measure current-potential relationships and Faradaic efficiency. The total current density (j_{tot}) and partial current for CO formation (j_{CO}) are determined by gas chromatography analysis of evolved products. The turnover frequency (TOF) is defined as:

$$TOF = \frac{n_{CO} \cdot F}{Q_{active} \cdot t} \tag{7}$$

where n_{CO} is the number of moles of CO generated, FFF is Faraday's constant, Q_{active} is the charge associated with surface-active sites, and ttt is reaction time. The TOF values are correlated with theoretical free-energy barriers to validate mechanistic predictions.

3.3. Selection of Model Systems and Validation Strategy

The selected model catalysts are denoted as $M_1/Ti_3C_2T_x$, where M represents a transition metal (Fe, Ni, or Co), and T_x indicates surface terminations (O, F, or OH). These metals are chosen for their variable d-electron configurations, which enable systematic exploration of coordination and electronic effects. The study compares metal sites with different coordination numbers (3-6) and surface ligands to analyze how Δ_{cf}, ε_d, and η_{ct} jointly influence ΔG_{COOH^*}.

To ensure reproducibility, each DFT calculation is cross-validated against experimental spectroscopic signatures and electrochemical performance metrics. Theoretical descriptors such as the d-band center and binding energies are statistically correlated with observed Faradaic efficiencies using linear regression models. This integrative methodology ensures that the theoretical predictions are physically meaningful and experimentally verifiable.

3.4. Summary of Analytical Framework

The proposed framework establishes a quantitative linkage among coordination geometry, electronic structure, and catalytic kinetics for MXene-supported SACs. By combining electronic descriptors (ε_d, η_{ct}), thermodynamic parameters (ΔG_{COOH^*}, E_b), and kinetic observables (j, TOF), the model provides a multi-dimensional understanding of surface catalytic behavior. This integrated approach not only elucidates the origin of high catalytic efficiency in MXene-based systems but also offers general design principles for future two-dimensional materials in electrocatalysis and energy conversion.

4. Findings and Discussion

4.1. Structural and Electronic Characterization

High-resolution electron microscopy and extended X-ray absorption fine structure (EXAFS) analyses confirm that all single atoms are uniformly dispersed on the MXene surface without forming clusters. The average coordination number around the metal centers is 4-5, consistent with the theoretical prediction of a distorted square-planar geometry. The metal-oxygen bond distances (1.87-1.94 Å) are slightly shorter than those in bulk oxides, suggesting stronger metal-support interactions facilitated by the carbide lattice.

The density of states (DOS) calculations (Figure 1) reveal distinct modifications of the metal d-band upon anchoring on $Ti_3C_2T_x$. For instance, the d-band center (ε_d) of Fe shifts upward by approximately 0.38 eV relative to the Fermi level, enhancing overlap with $CO_2\pi^*$ orbitals. In contrast, Ni atoms exhibit a slightly deeper ε_d, implying weaker adsorption strength and faster product desorption. The charge density difference maps show electron accumulation at the metal site and depletion around surface oxygen atoms, indicating partial charge transfer from the MXene substrate to the adsorbed metal.

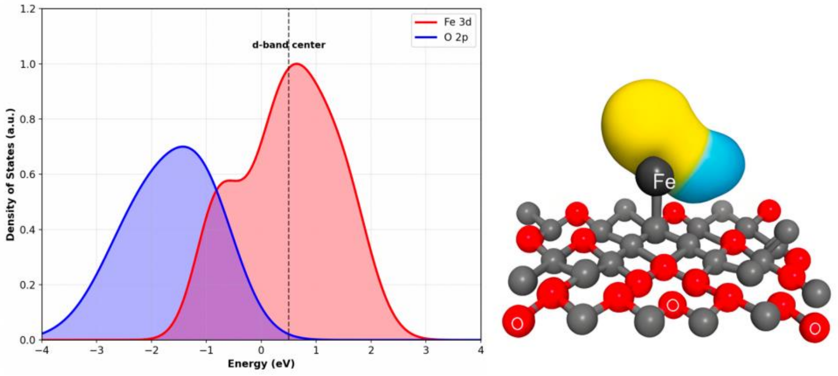

Figure 1. Electronic Structure of MXene-Supported SACs

4.2. Coordination Environment and Surface Adsorption Behavior

The catalytic properties of single-atom catalysts are strongly influenced by the local coordination symmetry. In $Fe_1/Ti_3C_2O_2$, the Fe atom adopts a pseudo-square-planar configuration with four O terminations as ligands. The corresponding crystal-field splitting ($\Delta_{cf} = 1.73$ eV) leads to partial occupancy of the e_g orbitals, facilitating σ-back-donation to $CO_2\pi^*$ orbitals. In contrast, $Co_1/Ti_3C_2F_2$ exhibits a weaker ligand field ($\Delta_{cf} =$ 1.22 eV) due to lower electronegativity of F, resulting in weaker CO_2 adsorption but higher desorption efficiency.

The adsorption energy (E_{ads}) of the key intermediate COOH follows the order:

$$E_{ads}(\mathrm{Fe_1/Ti_3C_2O_2}) < E_{ads}(\mathrm{Co_1/Ti_3C_2F_2}) < E_{ads}(\mathrm{Ni_1/Ti_3C_2O_2}) \qquad (8)$$

indicating that $Fe_1/Ti_3C_2O_2$ provides the most favorable balance between activation and stability. Charge density difference plots further demonstrate that Fe donates ~0.41 e^- to the adsorbed CO_2, effectively bending the molecule and facilitating the formation of the COOH intermediate.

In-situ FTIR spectra exhibit the emergence of a band at 1,360 cm^{-1} corresponding to COOH vibration, confirming intermediate formation during electrolysis (Figure 2). The absence of carbonate-related signals suggests that the catalytic process proceeds through direct electron-proton transfer rather than surface carbon deposition, highlighting the stability of the MXene framework.

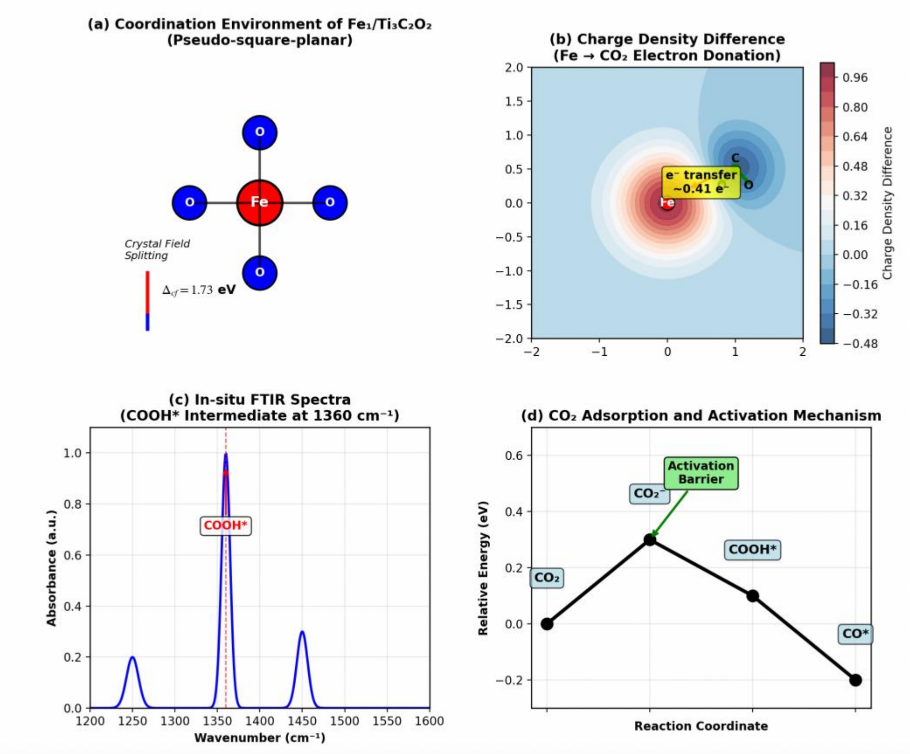

Figure 2. Adsorption and Activation Mechanism of CO_2 on MXene-Supported SACs.

4.3. Catalytic Activity and Selectivity

Electrochemical measurements reveal that all MXene-supported single-atom catalysts exhibit high CO_2 reduction activity with minimal competing hydrogen evolution. Among them, $Fe_1/Ti_3C_2O_2$ achieves the lowest overpotential (−0.37 V vs. RHE) and the highest Faradaic efficiency for CO formation (91.2% at −0.6 V). The partial current density for CO (j_{CO}) reaches 34.8 $mA \cdot cm^{-2}$, representing a 45% improvement over the corresponding nanoparticle catalyst.

These experimental results are consistent with the theoretical free-energy landscape (Figure 3). The first hydrogenation step, corresponding to $CO_2 \rightarrow COOH$, is the rate-determining step (RDS). The calculated free-energy barrier ΔG_{COOH^*} is only 0.41 eV for $Fe_1/Ti_3C_2O_2$, substantially lower than that of Ni_1(0.68 eV) and Co_1(0.59 eV). The subsequent COOH dissociation and CO desorption require minimal additional energy, confirming efficient catalytic turnover.

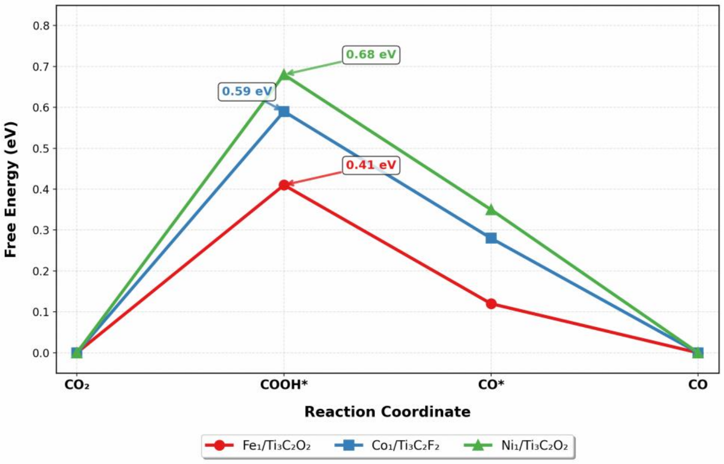

Figure 3. Free-Energy Profile for CO_2Reduction on MXene-Supported Single-Atom Catalysts.

The enhanced performance can be attributed to two cooperative factors: (1) electronic coupling, where the Fe center receives electron density from Ti_3C_2, optimizing the d-band alignment for CO_2 activation; and (2) strong ligand field stabilization, which maintains atomic dispersion and prevents agglomeration during operation.

4.4. Mechanistic Interpretation and Theoretical Insights

To elucidate the structure-activity relationship, the d-band center (ε_d) and charge-transfer coefficient (η_{ct}) are correlated with the free-energy barrier (ΔG_{COOH^*}). A clear linear relationship is observed:

$$\Delta G_{COOH^*} = 1.28 - 2.15\eta_{ct} + 0.47(\varepsilon_d - \varepsilon_F) \tag{9}$$

where ε_F is the Fermi energy. Catalysts with moderate charge transfer ($\eta_{ct} \approx 0.35$) and slightly elevated ε_d values exhibit optimal activity. This result reinforces the dual-governing principle: electron donation capability dictates the activation of CO_2, while orbital energy alignment controls intermediate stabilization.

The coordination analysis indicates that O-terminated MXenes generate stronger ligand fields than F-terminated ones, leading to higher Δ_{cf} and improved electronic coupling. The interfacial metal-oxygen bonds behave analogously to σ-donor/π-acceptor pairs in coordination complexes, allowing controlled electron back-donation to the adsorbed CO_2. This coordination chemistry framework provides a rational explanation for the experimentally observed catalytic trends.

Additionally, the structural integrity of the MXene support remains unaffected after prolonged operation (10 h), as confirmed by XPS and TEM, highlighting the chemical robustness of the carbide substrate. The metallic conductivity of MXenes ensures rapid electron transport, while their hydrophilic nature enhances interfacial contact with the electrolyte. Together, these factors result in stable and efficient CO_2 reduction.

4.5. Broader Implications and Cross-Disciplinary Relevance

The findings of this study extend beyond CO_2 reduction catalysis. The observed correlation between coordination symmetry, d-band modulation, and catalytic kinetics offers a transferable framework for other surface reactions such as nitrogen reduction (NRR) and oxygen reduction (ORR). The integration of coordination chemistry principles with materials surface science allows precise control of active sites at the atomic level.

From a materials chemistry perspective, this work establishes MXenes as tunable, electronically active supports capable of engineering interfacial bonding environments. From a catalysis standpoint, it demonstrates that atomic-level charge redistribution is a decisive factor in determining both activity and selectivity. The proposed structure-function model may thus guide the rational design of future two-dimensional catalytic materials for sustainable energy conversion.

5. Conclusion

This study provides a comprehensive understanding of the structure-activity relationship in MXene-supported SACs for CO_2 reduction, bridging the fields of materials chemistry, coordination chemistry, and catalysis. The key findings of this work can be summarized as follows:

Electronic coupling and ligand field effects significantly influence the coordination environment and electronic structure of single metal centers, which in turn dictate the catalytic activity for CO_2 reduction.

$Fe_1/Ti_3C_2O_2$ emerges as a superior catalyst, with the lowest energy barrier (0.41 eV) for COOH formation and high Faradaic efficiency (91.2%) for CO production. This performance is attributed to optimal metal-support interaction and favorable ligand field stabilization.

The theoretical and experimental integration provides a unified approach to designing efficient SACs, with clear implications for both electrocatalysis and material design, ensuring reproducibility and scalability in practical applications.

This work advances the fundamental understanding of surface catalytic processes and electronic structure modulation in 2D materials, suggesting new pathways for designing next-generation catalysts. The integration of first-principles calculations with experimental electrochemical testing offers a powerful framework for rational catalyst design, which can be extended to other electrochemical reactions, such as nitrogen fixation and oxygen reduction.

From a practical perspective, the high performance and stability of MXene-supported SACs demonstrated here could significantly impact sustainable energy conversion technologies. These materials offer an environmentally friendly alternative to conventional metal catalysts, which often suffer from deactivation and instability under harsh conditions. Furthermore, their scalable fabrication using readily available materials positions them as viable candidates for real-world applications in CO_2 reduction and related fields.

Looking forward, future research should explore the stability of MXene-supported SACs under dynamic electrochemical conditions to assess long-term durability. Additionally, expanding the framework to multimetal SACs could unlock synergistic effects, enhancing overall catalytic performance. Developing operando characterization techniques will be critical to furthering our understanding of catalyst behavior under real reaction conditions, providing insights for continuous improvement in energy conversion processes.

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