

A standardized dataset of CO-TPD spectra on transition-metal single-crystal surfaces

YANG Lin¹, WU Jianghong², WANG He^{3,*}

¹School of Statistics, Shanxi University of Finance and Economics, Taiyuan 030006, China;

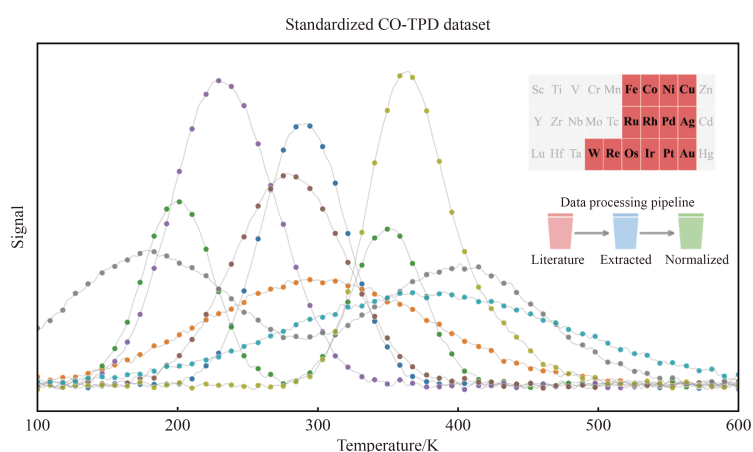
²Department of Energy Chemistry and Materials Engineering, Shanxi Institute of Energy, Jinzhong 030600, China;

³Institute of Coal Chemistry, Chinese Academy of Sciences, State Key Laboratory of Coal Conversion, Taiyuan 030001, China

Abstract: Temperature-programmed desorption (TPD) is a fundamental technique in surface science and heterogeneous catalysis for characterizing adsorption behavior, and for extracting key parameters such as adsorption energy. However, the majority of existing TPD data is accessible in the form of published images, which lacks structured and quantitative datasets. This constrains its utility for rigorous quantitative analysis and computational modelling. Using carbon monoxide (CO) which is a widely adopted probe molecule, a curated and

standardized dataset of CO-TPD is constructed, encompassing 14 transition-metal single-crystal surfaces, including copper (Cu) and ruthenium (Ru). By systematically extracting numerical data points from published spectra and applying normalization, essential spectral features such as peak shape are fully preserved. The dataset also documents relevant experimental parameters, including heating rates, and was developed using a standardized protocol for data collection and quality control. This resource serves as both a reference library to support the deconvolution of TPD spectra from complex catalysts and an experimental benchmark for calibrating parameters in theoretical models. By providing a reliable and accessible data function, this work advances the microscopic understanding and the rational design of catalyst active centers.

Key words: CO-TPD; standardized dataset; transition metal; single-crystal surfaces



Temperature-programmed desorption (TPD) is a fundamental technique for characterizing surface adsorption processes. By heating a sample pre-adsorbed with probe molecules (e.g., CO, H₂) at a constant rate and monitoring the desorption signal as a function of temperature, TPD provides access to key physicochemical properties of material surfaces. Systematic analysis of desorption peak positions, shapes and intensities, and how these evolves with coverage, allows for the extraction of critical parameters, such as desorption energy, types of adsorption states, surface coverage, and the reaction kinetics of

adsorbed species. Therefore, TPD plays an indispensable role in surface science and heterogeneous catalysis research.

Carbon monoxide (CO) is both a widely used probe molecule and a key intermediate in numerous catalytic reactions. It has therefore been extensively studied for its adsorption and desorption behavior on transition metal surfaces. This stems from two factors: the relatively simple and readily detectable structure of the CO molecule and its ability to form diverse adsorption configurations, such as adsorption at linear, bridge, and hollow sites. These configurations are highly sensitive to the electronic

Received: 2025-12-04; Revised: 2025-12-28

Foundation items: Supported by the Robotic AI-Scientist Platform of Chinese Academy of Sciences, National Natural Science Foundation of China (22372185), Youth Talent Development Program of SKLCC (2025BWZ009), Natural Science Foundation of Shanxi Province (202203021221219), Research on the Construction of Scientific and Technological Innovation Think Tank of Shanxi Association for Science and Technology (KXKT202542).

* Corresponding author. Tel: 19946235450, E-mail: wanghe@sxicc.ac.cn.

DOI: 10.1016/S1872-5813(26)60673-1 CSTR: 32157.14.2097-213X.2026.JFCT.0029 Associated Data DOI: 10.57760/sciencedb.32906

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structure and local coordination environment of the metal surface. Consequently, a precise analysis of CO-TPD spectra can directly reveal the bonding strength between CO and the surface, the distribution of adsorption sites, and intermolecular interactions. This provides an essential experimental foundation for understanding catalytic reaction mechanisms and the rational design of efficient catalysts.

Despite the extensive study of CO-TPD experiments on various transition metal single-crystal surfaces, the analytical potential of these valuable data remains largely untapped, primarily due to three major challenges. First, data is often presented solely in graphical form, which results in a lack of digitally accessible numerical datasets. This leads to the loss of critical information such as complete peak shapes and precise intensities, which severely hinders quantitative analysis. This issue is exacerbated by analytical limitations in complex systems, where current methods that rely on peak temperature for qualitative site assignment are unable to accurately deconvolute the broad and overlapping signatures typical of nanoparticles or alloys. This prevents the quantitative discrimination of distinct active sites. Furthermore, there is a significant gap between theory and experiment, as simulations struggle to replicate detailed spectral features like peak shape and asymmetry. This is largely due to the scarcity of highly-fidelitous and complete peak-profile data required to calibrate key theoretical parameters such as coverage-dependent adsorption energies and intermolecular interactions.

This study aims to bridge these gaps by constructing a

systematic and quantitative CO-TPD reference dataset. We used WebPlotDigitizer^[1] for digitization and applied stringent normalization procedures to preserve complete peak profiles alongside key experimental parameters covering 14 common transition metals across various single-crystal surfaces, including Ag^[2], Au^[3–5], Co^[6–10], Cu^[11–21], Fe^[22–30], Ir^[31–37], Ni^[38–48], Os^[49], Pd^[50–62], Pt^[45,63–88], Re^[89], Rh^[57,90–97], Ru^[89,98–103], and W^[104–106]. The resulting dataset establishes a well-structured reference spectral library. It supports the deconvolution of TPD profiles from complex catalysts and provides a benchmark for calibrating theoretical models, thereby bridging the gap between experiment and computation in surface science and catalysis. While CO-TPD is also valuable for studying oxides, alloys, and single-atom catalysts, data from these systems often lack standardization and quantitative consistency. The current dataset on well-defined transition-metal surfaces provides a foundational reference that will support the future development of standardized and interpretable datasets for more complex catalytic materials.

1 Main part

1.1 Data profile

Table 1 systematically summarizes the basic information of the standardized dataset of CO-TPD spectra on transition-metal single-crystal surfaces, covering key metadata such as the author's information, data description, generation time, file formats, and access sources.

Table 1 Dataset basic information of CO-TPD spectra on transition-metal single-crystal surfaces

Data title (V0.1)	A standardized dataset of CO-TPD spectra on transition-metal single-crystal surfaces
Author's name	YANG Lin, WU Jianghong, WANG He
Corresponding author's name	WANG He
Data content description	This data set consists of 14 parts, including adsorbed species, surface, references (DOI), initial temperature (K), pre-adsorption conditions, heating rate (K/s), spectral peak position, type of peak, temperature measurement method, baseline quality, original TPD figure, other detection methods in the literature, scaled TPD data points, and data points obtained from TPD diagram. Among them: (1) TPD list.csv, as the core index file, can directly read the first 10 basic parameters and "other detection methods in the literature", while the rest should be read from TPDdata.zip and TPDdata_scaled.zip based on the path given in TPD list.csv. The data volume of TPD list.csv is 84.3 KB; (2) TPDdata.zip contains "original TPD figure" and "data points read from TPD diagram", providing the original spectral image extracted from the literature and the original coordinate data directly collected through WebPlotDigitizer software without scaling processing, with a data volume of 11.4 MB; (3) TPDdata_scaled.zip provides "scaled TPD data points", i.e., the standardized data points after normalization processing based on the maximum peak of each spectral map, which is convenient for the comparison of spectral shape and intensity across literature and experimental conditions, with a data volume of 645 KB.
Data generation time	1976—2023
Data volume	717 entries/13.7 MB
Data format	.zip, .csv
Data source location	http://www.dx.doi.org/10.57760/sciencedb.32906
Citation format of data	YANG Lin, WU Jianghong, WANG He. A standardized dataset of CO-TPD spectra on transition-metal single-crystal surface[J]. J Fuel Chem Technol, 2026, 54, 20250388. YANG Lin, WU Jianghong, WANG He. A standardized dataset of CO-TPD spectra on transition-metal single-crystal surfaces[DS/OL]. Science Data Bank, 2026. https://doi.org/10.57760/sciencedb.32906 . DOI: 10.57760/sciencedb.32906.

1.2 Data value

The primary significance of this dataset is that it advances TPD analysis from merely focusing on “peak temperature” to comprehensively examining “peak shape”. By providing complete spectral data points, the dataset enables the extraction of key parameters such as full width at half maximum (FWHM), peak shape, and peak intensity. Thereby, it reveals finer details about the energy distribution of adsorption sites. Furthermore, the dataset systematically incorporates spectra from various transition metals across flat to stepped crystal planes, and provides a continuous profile to help understand how surface structure influences adsorption behavior. This structured spectral library supports the deconvolution of TPD profiles from complex catalysts such as nanoparticles and alloys, and serves as an experimental benchmark for calibrating and validating theoretical models. These functions also bridge the gap between experimental observation and computational prediction, facilitating the transition from qualitative interpretation to quantitative analysis in surface science and catalysis research.

To demonstrate the practical application value of this dataset, a case study is presented focusing on nickel (Ni) nanoparticle surfaces, which are commonly used in heterogeneous catalysis and which typically exhibit multiple crystal facets. Under identical experimental conditions (saturation adsorption at 100 K and a heating rate of 2 K/s), the CO-TPD spectra of the Ni(111) and Ni(100) single-crystal surfaces in our dataset exhibit similar desorption peak temperatures (330 and 425 K for Ni(111), and 325 and 420 K for Ni(100)). However, there are systematic differences in the shape of the peaks: the Ni(111) desorption peaks are narrower and more symmetric, whereas the Ni(100) peaks show distinct broadening on the low-temperature side (as the black and navy lines for (111) and (100) shown in Figure 1). Using these normalized spectra as “fingerprint” references, a linear combination fitting approach can deconvolute the broad, overlapping TPD profiles of Ni nanoparticles. By adjusting the weight ratios of the Ni(111) and Ni(100) components, the composition of the surface facets can be estimated semi-quantitatively (as illustrated in Figure 1). This approach goes beyond traditional peak-temperature analysis, offering a more reliable basis for linking surface structure to catalytic performance in complex nanoparticle systems.

1.3 Data generation method or process

The construction of this dataset involves a systematic workflow, encompassing a literature search and screening, data extraction, numerical conversion, and preprocessing involving baseline correction and normalization, as summarized in Figure 2. Relevant publications were first identified through keyword searches (e.g., “CO TPD on Cu(111)”, “CO adsorption on Pt”, etc.). The reference lists and citation networks of the initially retrieved papers were then examined to expand the collection with additional

high-quality sources, including journal articles and dissertations. During the screening process, priority was given to studies containing CO-TPD data from well-defined single-crystal surfaces that explicitly specified the heating rate (either directly or *via* referenced sources) and provided well-described spectral data. This ensured the reliability and comparability for subsequent processing. For the selected TPD spectra, the graphical data were digitized using the software WebPlotDigitizer to extract the original coordinate points. This step was performed manually to ensure precision and to avoid errors that automated tools might introduce when interpreting complex or overlapping spectral features. Each profile was independently and accurately converted into a numerical dataset. Following data extraction, key preprocessing steps were applied, including baseline correction and normalization. Baseline correction was conducted by identifying the minimum signal value $I_{\min}$ within the non-desorbing temperature regions (typically at the low- or high-temperature ends of the spectrum) and subtracting this value from all data points in the curve, thereby resetting the baseline to 0. This process effectively removes background signal offsets while preserving the intrinsic spectral shape. To address variations in signal intensity units and scaling factors across different studies, normalization was carried out based on the maximum peak height, $I_{\max}$. The normalized intensity value for each data point was calculated using the following equation:

$$I_i^{\text{norm}} = \frac{I_i - I_{\min}}{I_{\max} - I_{\min}} \quad (1)$$

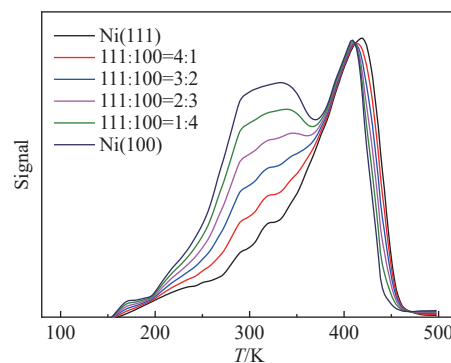


Fig. 1 Comparative CO-TPD spectra for Ni(111), Ni(100), and mixed-composition surfaces with different (111)/(100) ratios, following 100 K saturation and a heating rate of 2 K/s

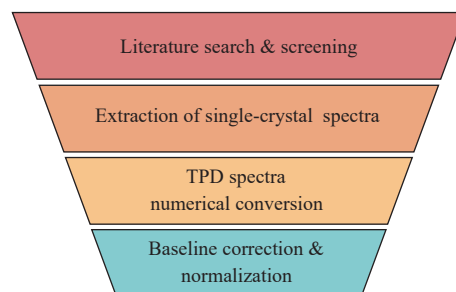


Fig. 2 Schematic of the data collection workflow

where I_i and I_i^{norm} are the original and normalized intensities at point i , respectively. This operation scales the signal range to between 0 and 1, which facilitates direct comparison of spectral shapes and relative intensities across different experimental setups. Specifically, for multiple curves within the same publication that share a common baseline, normalization is performed relative to the highest peak in the curve corresponding to the maximum adsorption coverage. For the case of different baselines, however, each curve was normalized individually. This approach preserves the relative intensity relationships among spectra obtained under varying experimental conditions within the same study, and provides a consistent basis for subsequent in-depth analysis and cross-study comparison. Please note that, all data used in this dataset are sourced from publicly available academic literature and each data entry in the dataset contains the complete digital object identifier (DOI) of the corresponding original publication to ensure traceability and transparency. Furthermore, the filenames of the original TPD figures follow a uniform naming convention in the format “JournalAbbreviation_Year_Volume_Page”, facilitating direct referencing to the source.

In addition to the TPD spectra, relevant metadata was systematically extracted from the literature to ensure comprehensive documentation and support subsequent analysis. This includes surface information such as the type of metal and its crystallographic orientation (e.g. Pt(111), Ag(221)). Key experimental parameters, such as the initial temperature, pre-adsorption conditions, heating rate, and temperature measurement method, were recorded, as they are essential for spectrum interpretation and theoretical model calibration. Spectral characteristics, such as peak position, peak type, and baseline quality, were also noted to

provide a preliminary understanding of each TPD spectrum. Additionally, any complementary analytical techniques reported in the same studies were compiled to enable multi-spectral correction and to support the interpretation of the TPD data.

1.4 Data sample description

The dataset includes CO-TPD spectra obtained from the single-crystal surfaces of 14 common transition metals, including Ag, Au, Co, Cu, Fe, Ir, Ni, Os, Pd, Pt, Re, Rh, Ru, and W. A total of 717 measurements were taken across these metals, covering a range of crystal planes from low-Miller-index facets, such as (111), (110), and (100), to stepped surfaces including (355) and (533). Each entry in the dataset contains 14 standardized parameters, with detailed descriptions provided in Table 2.

To provide an overview of CO desorption properties across different transition-metal surfaces, Table 3 summarizes the typical temperature ranges of CO desorption peaks under low-coverage conditions for several single-crystal surfaces. It should be noted that the data was collected from studies conducted under different experimental setups, particularly with regard to heating rates, which precludes a strictly uniform comparison across all systems. Therefore, the temperature ranges provided here are intended as indicative references rather than absolute values. The low-coverage data was selected for its closer reflection of the intrinsic metal-CO interaction, as intermolecular effects are minimized under these conditions.

Table 2 The parameters of each TPD entry and their description

Parameter	Description
Adsorbed species	it mainly includes CO and its relative isotopes, such as C^{13}O and CO^{18}
Surface	metal name and Miller indices, such as Ag(221)
Reference (DOI)	literature sources of data, including DOI or URL (including dissertations)
Initial temperature	pre-adsorption temperature in temperature programmed desorption, in K
Pre-adsorption condition	conditions or coverage of pre-adsorbed gas species, in units of molecules/cm ² , L, mbar·s, or ML
Heating rate	heating rate in temperature programmed desorption, in K/s
Spectral peak position	spectral peak positions reported in the literature, or extracted directly from spectral data points (if not mentioned in the text), in K
Type of peak	they are mainly categorized into three types: single peaks, step-like peaks, and hump-shaped peaks. Examples of step-like peaks and hump-shaped peaks are shown in Figure 3
Temperature measurement method	Sample or sample holder. If temperature is measured directly on the sample, it indicates higher accuracy; if measured <i>via</i> the sample holder, it implies certain measurement errors that require attention
Baseline quality	good or poor. A good baseline indicates more reliable results
Original TPD figure	image location of the TPD spectrum extracted from the literature
Other detection methods in the literature	other characterization or analytical techniques employed in the same article to assist TPD analysis
Scaled TPD data points	storage location of the scaled TPD data
Data points extracted from TPD figures	storage location of TPD data points generated <i>via</i> WebPlotDigitizer software

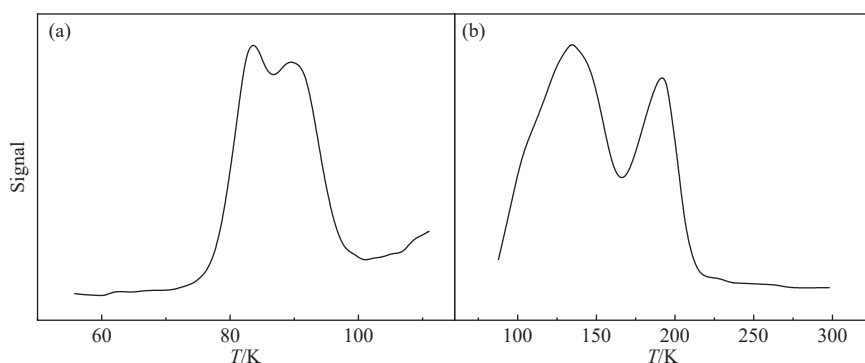


Fig. 3 Schematic diagrams of two TPD peak shapes: (a) step-like peak and (b) hump-shaped peak

Table 3 Typical CO desorption temperature ranges for corresponding single-crystal surfaces under low-coverage conditions

Surface	Range of desorption temperature/K	Surface	Range of desorption temperature/K
Ag(221)	90	Pd(100)	490
Au(211)	190	Pd(112)	465–510
Au(111)	95	Pd(110)	494–502
Co(0001)	415–430	Pd(111)	485–511
Co(10-10)	405	Ru(0001)	475–490
Fe(110)	800	Ru(10-10)	520
Fe(111)	760	Ru(10-19)	473
Ir(110)	614	Pt(100)	475
Ir(111)	525–550	Pt(111)	435–490
Ir(100)	565	Pt(110)	500–530
Ir(211)	670	Pt(112)	500–504
Ni(111)	410–450	Rh(111)	500–540
Ni(100)	420–435	Rh(100)	500
Ni(110)	445	Rh(110)	485–500
Ni(551)	460	Rh(210)	468
Os(0001)	525	Cu(100)	183–208
W(110)	300	Cu(110)	206–218
W(100)	330	Cu(111)	173–189

Table 3 shows some general trends: for instance, CO desorbs at relatively low temperatures (typically below room temperature) from Cu, Ag, and Au surfaces, whereas desorption from W occurs slightly above room temperature; Co, Ni, Pd, and Pt exhibit desorption peaks in the range of 400–500 K, and Ru, Rh, Os, Ir, and Fe generally show desorption temperatures above 500 K. These trends are consistent with the known variations in metal–CO bond strengths reported in the literature. More detailed spectral features and complete experimental parameters can be accessed in the dataset file “TPD list.csv”.

1.5 Data quality

To ensure the accuracy and reliability of the dataset, a series of rigorous quality control measures were implemented throughout its construction. Wherever

possible, each TPD entry was paired with complete experimental metadata, and only data obtained from clean single-crystal surfaces were included. This excluded those involving pre-adsorption of other species or doped metal surfaces. In cases of incomplete information, relevant parameters were annotated explicitly (e.g. heating rates as “~5 K/s” or doses as “<12 L”). Furthermore, extracted desorption peak temperatures were cross-verified against values in the literature to ensure consistency. To preserve physically realistic curve profiles and enhance data integrity, key regions of the spectra, particularly near peak features, were refined by carefully increasing the number of data points where the original digitization yielded sparse data points. Anomalous fluctuations resulting from overlapping curves or extraction artifacts were also removed. The credibility of each spectrum was also assessed based on baseline quality, which served as an

indicator of overall reliability. These procedures result in a dataset comprising 478 high reliability entries, which feature good baselines, clearly defined heating rates and pre-adsorption conditions, and direct sample temperature measurement. Additionally, 239 entries of lower reliability are also included. While the latter exhibit greater uncertainty, they remain valuable for identifying surface-active sites and for probing their interaction with CO, and they may also gain reliability through further calibration or integration complementary theoretical calculations.

To further enhance and refine this dataset, we will make improvements in three key aspects. First, we will expand the dataset by incorporating CO-TPD data from single-crystal surfaces that are not currently included, such as metallic oxides (e.g. MgO(100)) and bimetallic systems (e.g. Pt/Ru(0001)). Second, we will use the robotic AI-Scientist platform of the Chinese Academy of Sciences to systematically perform CO-TPD experiments on published surfaces and then apply a unified data processing protocol to minimize errors arising from manual operations and inconsistencies due to varying methodologies across studies. Third, we will integrate theoretical prediction spectra alongside their model parameters, thereby significantly improving the dataset's usability and comprehensiveness. These updates will be tracked *via* the ScienceDB project page.

1.6 Data usage methods and suggestion

This dataset offers multi-level application support for research in surface science and heterogeneous catalysis. Firstly, it allows users to extract basic data and to analyze feature directly from the structured metadata file. By referencing the provided TPD list.csv, users can locate critical experimental parameters such as heating rates, the desorption peak positions, and pre-adsorption conditions. They can then access the corresponding spectral data files, which allows them to quantitative characterization of peak features, including the full width at half maximum, peak symmetry and integrated intensity.

Secondly, the dataset enables the quantitative or semi-quantitative analysis of complex catalyst surfaces. When studying nanoparticles or alloys, whose CO-TPD spectra typically exhibit broadened or overlapping desorption peaks, the normalized single-crystal spectra in this dataset, such as Pt(111), Pt(100), Pt(211) and Pt(410), can be used as reference components for spectral deconvolution. A practical workflow includes: locating the relevant scaled TPD data points for specific surfaces from the TPD list.csv file; extracting the numerical data points from the provided csv files with Origin or Python; applying smoothing and interpolation routines to enhance data continuity; using the Redhead equation^[107] to convert the desorption profiles to the concerned heating rate; and performing linear combination or peak-fitting against the experimental TPD

curve of a complex catalyst. This approach goes beyond traditional qualitative peak assignments, quantifying the distribution and contribution of distinct active sites (e.g. terraces, steps, kinks) and offering a more precise experimental basis for structure-activity relationship studies. A representative example can be found in the work of Wong et al.^[108], where the experimental CO₂-TPD profile of a stepped Pt(997) surface was deconvoluted using simulated TPD spectra from Pt(111), Pt(221) and Pt(965) surfaces, enabling site-specific quantification.

Thirdly, the dataset provides a high-fidelity experimental benchmark for calibrating and optimizing theoretical models. Integrating first-principles calculations and microkinetic simulations establishes a systematic calibration workflow that bridges the gap between computational predictions and experimental observations. Specifically, adsorption energies obtained from DFT calculations and sticking coefficients are used to generate simulated TPD profiles *via* microkinetic modelling. To align these simulated spectra with experimental TPD profiles from the dataset, correction factors or parameterized correction functions can be introduced for adsorption energies and sticking coefficients. It is noteworthy that simultaneous fitting of multiple TPD curves measured under different coverages and conditions can be incorporated into the optimization process, which is crucial for enhancing the transferability of the calibrated model. Optimization algorithms such as genetic algorithms or Bayesian optimization can then be employed to adjust these corrections iteratively by minimizing the multi-spectral discrepancy between the simulated and experimental TPD line shapes (including peak temperature, width, asymmetry, and the overall profile). This multi-condition calibration strategy improves the agreement with known systems and significantly enhances the model's predictive capability for unknown surfaces, thereby advancing theoretical predictions from “where desorption occurs” to “how desorption proceeds” across a wide range of experimental scenarios.

Furthermore, the dataset serves as a valuable teaching resource for surface science and catalysis courses, and allows instructors to illustrate concepts such as structure sensitivity and desorption kinetics by making systematic spectral comparisons. Thanks to its structured, well-annotated format, the dataset also forms an ideal foundation for developing machine-learning models that correlate spectral features with surface structure. This opens up a data-driven pathway for catalyst screening and rational design.

2 Conclusion

This study presents a systematically compiled CO-TPD dataset that transforms fragmented graphical data into complete, digitized spectral profiles. This shifts the focus of

traditional analysis from isolated “peak temperatures” to integrated, digitized “complete spectral profiles”.

For experimental catalysis, this dataset serves as a reference library for deconvoluting spectra from complex catalysts, enabling semi-quantitative site-specific analysis. In theory, it provides a high-fidelity benchmark for inverse-calibrating coverage-dependent adsorption parameters *via* full-profile matching, thereby enhancing model reliability. Furthermore, the dataset has educational value in teaching surface-science concepts, and supports machine-learning approaches by providing structured data to correlate surface structure with spectral features.

In summary, this dataset bridges the gap between modelling and real-world catalysis by connecting experimental observations with theoretical understanding to accelerate progress in the microscopic analysis and rational design of catalyst active sites. Expanding the dataset to include oxides, bimetallic alloys, and single-atom systems—along with integrated theoretical spectra—will further enhance its utility as a comprehensive reference for deciphering adsorption behavior across diverse catalytic surfaces.

Data availability statement

The data supporting the results in this study has been published in sciencedb database and can be obtained through DOI: 10.57760/sciencedb.32906.

Declaration of Competing Interest

The authors declare no conflict of interest.

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过渡金属单晶表面 CO-TPD 谱图的标准化数据集

杨 琳¹, 武江红², 王 鹤^{3,*}

(1. 山西财经大学统计学院, 山西 太原 030006; 2. 山西能源学院 能源化学与材料工程系, 山西 晋中 030600;

3. 中国科学院山西煤炭化学研究所 煤炭高效低碳利用全国重点实验室, 山西 太原 030001)

摘 要: 程序升温脱附(TPD)是表征表面吸附行为的关键实验技术, 能够获取吸附能等关键参数, 在多相催化研究中具有广泛应用。然而, 现有 TPD 数据多以图像形式呈现, 缺乏系统、数值化的数据集, 限制其定量分析与理论建模的潜力。CO 作为典型探针分子, 其 TPD 谱图可用于识别表面活性位点, 是研究金属表面性质的有效手段。本研究构建了一个涵盖 Cu、Ru 等 14 种过渡金属单晶表面的 CO-TPD 数据集。通过提取文献谱图的数值点并进行归一化处理, 完整保留了峰形等关键信息。数据集中还包含升温速率等实验参数, 并建立了标准化的数据采集与质量控制流程。该数据集不仅可作为“指纹谱图库”用于复杂催化剂 TPD 谱图解卷积, 还可作为实验基准, 用于理论模型的参数校正。本工作为表面科学与催化研究提供了可靠的数据基础, 有助于催化剂活性中心的微观解析与理性设计。

关键词: CO-TPD; 标准化数据集; 过渡金属; 单晶表面

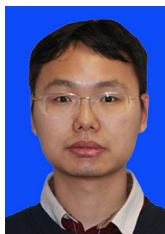
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作者简介:



杨琳(1989), 博士, 主要从事生存分析理论方法研究和深度学习、机器学习等统计方法的改进与应用, ylintj@126.com。



王鹤(1990), 男, 博士, 副研究员, 主要从事多相催化的理论模拟及动态实验谱图的微观理论解析研究, wanghe@sxicc.ac.cn。