

A computational dataset for C1 molecules catalytic conversion over iron-based catalysts

ZHANG Jian¹, LI Chaochao¹, LU Kuan^{2,*}

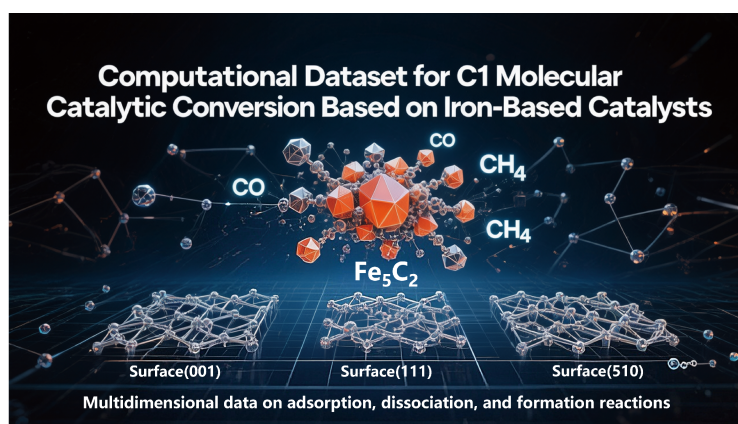
¹School of Statistics, Shanxi University of Finance and Economics, Taiyuan 030006, China;

²Institute of Coal Chemistry, Chinese Academy of Sciences, State Key Laboratory of Coal Conversion, Taiyuan 030001, China

Abstract: The catalytic conversion of C1 molecules (e.g., CO, CO₂) represents a pivotal technology in the energy and chemical sectors, essential for achieving sustainable C1 chemistry and low-carbon transformation. A profound understanding of the underlying microscopic reaction mechanisms necessitates systematic support from both theoretical and experimental data support. This study constructs a “Computational Dataset for C1 Molecular Catalytic Conversion Based on Iron-Based Catalysts,” focusing on

Fe₅C₂-based catalysts and systematically integrating multidimensional information on C1 molecular adsorption, dissociation, and formation reactions across different crystal surfaces (001, 111, 510). The dataset includes: the number of polycrystalline surface structures (Fe₅C₂(001) with 96 configurations, Fe₅C₂(111) with 93, and Fe₅C₂(510) with 472); species involved in the full reaction pathways under complex co-adsorption environments (adsorbed states such as COH and H₂, dissociated states like CO under 2H conditions, and formation states such as CH/CH₃ under 2H and H₂O conditions); and a standardized hierarchical storage system categorizing reaction types, crystal surfaces, and structural parameters. This dataset not only serves as a benchmark for validating quantum chemical calculation methods but also provides critical data support for catalyst design and reaction pathway optimization in C1 molecular catalytic conversion by uncovering the coupling effects of crystal surfaces and reaction mechanisms.

Key words: Fe₅C₂; C1 molecules; density functional theory; reaction mechanism; dataset



The catalytic conversion of C1 molecules (such as CO, CO₂, etc.) is central to industrial processes like syngas production, methane reforming, and the water-gas shift reaction, holding strategic significance for energy structure transformation under carbon neutrality goals. However, the elementary reactions of C1 molecules on catalyst surfaces—such as adsorption, dissociation, and recombination—are regulated by the coupling of multiple factors, including crystal facet structure, active sites, and reaction environments. Elucidating these microscopic mechanisms has long faced two major challenges: first, limitations in experimental characterization make it difficult

to capture atomic-level structures and electronic states in real-time during dynamic reactions, hindering the full revelation of reaction pathways; second, existing quantum chemical calculations mostly focus on single crystal facets or isolated reaction stages, lacking multidimensional and systematically integrated datasets. Among various catalytic materials, iron-based catalysts have attracted significant attention due to their low cost and excellent catalytic performance, with χ -Fe₅C₂^[1–3] being widely regarded as the main active phase in Fischer-Tropsch synthesis. Research indicates that the Fe₅C₂(510) surface^[3–4] is the most representative catalytic interface for Fischer-Tropsch

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* Corresponding author. E-mail: lukuan@sxicc.ac.cn.

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synthesis, exhibiting high CO activation activity and C–C coupling ability.

The paper aims to the “Computational Dataset for Catalytic Conversion of C1 Molecules on Iron-Based Catalysts,” which systematically collects key parameters such as adsorption energies and reaction barriers for various surface configurations, adsorption sites, and coverages in interaction systems involving different surfaces of iron-based catalysts. The construction of this dataset is of paramount necessity for several reasons: Firstly, it addresses the limitations of existing studies that focus on single crystal facets or isolated reaction steps by providing multidimensional data covering the entire reaction cycle. Secondly, compared to general-purpose databases like Material Project, its targeted design focusing on the Fe_5C_2 catalytic system can more precisely align with the needs of C1 conversion mechanism research and catalyst development. This data paper aims to provide a detailed description of the dataset’s generation process, content structure, quality control methods, and application value, offering reliable data support and theoretical guidance for researchers in related fields. By sharing these high-quality quantum chemical calculation data, we aim to enhance the understanding of catalytic conversion of C1 molecules on iron-based Fischer-Tropsch catalysts and accelerate the development of efficient catalyst designs and novel carbon cycle technologies.

1 Main part

1.1 Data profile

The full name of this dataset is “Computational Dataset for Catalytic Conversion of C1 Molecules Based on Iron-Based Catalysts,” with version number V1.0. The dataset centers on the 001, 111 and 510 crystal planes of Fe_5C_2 as the core research subjects, covering three fundamental reactions of C1 molecules on the catalyst surface:

adsorption, dissociation, and formation (Table 1). It relies on density functional theory to obtain structural and energy parameters. The directory structure is hierarchically organized, with clear data architecture, and file naming reflects the reaction system, pathway, and type, facilitating user identification and retrieval.

1.2 Data value

From a theoretical perspective, this dataset systematically stores high-precision computational data (such as adsorption energies, dissociation barriers, and product distributions) for the complete reaction pathways of C1 molecules on multiple crystal facets (001, 111, 510) of Fe_5C_2 , providing abundant case studies for investigating the synergistic adsorption mechanisms of C/H/O. The cross-facet and multi-reaction comparative analyses within the dataset can further reveal the intrinsic relationship between crystal facet effects (e.g., step density, atomic coordination number) and reaction selectivity, advancing C1 catalytic conversion theory from single-facet studies toward multidimensional mechanistic coupling.

Regarding catalyst design, the energy and structural parameters in the dataset can be directly used to establish reaction kinetic models and predict product selectivity under different reaction conditions. Research shows that the presence of surface OH groups can significantly alter the product distribution of iron-based catalysts and enhance olefin selectivity^[5]. This dataset provides a theoretical basis for the rational design of surface-modified Fe_5C_2 catalysts by detailing the influence of water molecules on the surface C/H ratio. For example, the results on how water molecules affect surface carbon coverage allows for the precise regulation of the active environment on the catalyst surface, thereby reducing the formation of undesired by-products like methane and increasing the production efficiency of higher-value products with longer carbon chains (C_{2+} , such as ethylene and propylene).

Table 1 Overview of basic information of dataset

Data title	Computational dataset for catalytic conversion of C1 molecules based on iron-based catalysts
Data version	V1.0 (released in December 2025)
Software version	VASP 5.3.5
Author’s name	ZHANG Jian, LI Chaochao, LU Kuan
Corresponding author’s name	LU Kuan
Data content description	The dataset focuses on the (001), (111) and (510) crystal planes of Fe_5C_2 , covering three fundamental reaction types: adsorption, dissociation, and formation of C1 molecules on the catalyst surface. Structural and energetic parameters are obtained based on density functional theory
Data generation time	2024—2025 year
Data volume	Approximately 1.4 GB (690 directories, 1961 files)
Data format	POSCAR, CONTCAR, OUTCAR
Data source location	CSTR:31253.11.sciencedb.34259. https://doi.org/10.57760/sciencedb.34259
Citation format of data	ZHANG Jian, LI Chaochao, LU Kuan. A computational dataset for C1 molecules catalytic conversion over iron-based catalysts[J]. J Fuel Chem Technol, 2026, 54, 20250429. LU Kuan. Computational dataset for catalytic conversion of C1 molecules based on iron-based catalysts [DS/OL]. V1. Science Data Bank, 2025[2025-12-23]. https://doi.org/10.57760/sciencedb.34259 . DOI:10.57760/sciencedb.34259.

At the methodological level, the dataset provides a high-quality computational benchmark for surface catalytic reactions, which can be used to validate the accuracy of computational methods or train machine learning force fields. The data includes nearly 700 optimized adsorption structures and reaction transition states, covering various chemical environments of elements such as C, O and H on the Fe_5C_2 surface, serving as reference data for surface catalytic reaction simulations. Additionally, the rich structure-energy correlations in the dataset offer training samples for developing rapid catalytic activity descriptors and machine learning models.

In terms of application prospects, the dataset covers multi-scenario reaction data across the entire cycle of C1 molecule conversion (adsorption $\rightarrow$ dissociation $\rightarrow$ formation), such as syngas-to- CH_4 and CO_2 catalytic conversion, directly serving the optimization of industrial catalytic processes. For example, by analyzing the HCOO formation pathway on the $\text{Fe}_5\text{C}_2(510)$ crystal surface in a “ $2\text{H}_2\text{O}+2\text{H}$ environment”, the impact of water conditions on CO_2 hydrogenation conversion can be investigated. Additionally, the correlation between environmental parameters (e.g., H_2O partial pressure) and product distribution in the dataset can guide the dynamic adjustment of operating conditions in industrial reactor designs (e.g., fluidized bed, fixed bed), facilitating breakthroughs in efficient carbon resource conversion and low-carbon emission technologies.

1.3 Data generation method or process

All calculations in this dataset were performed based on density functional theory using the Vienna Ab initio Simulation Package (VASP) software^[6-7]. The projector augmented wave (PAW) pseudopotential^[8] was employed to describe the atomic nuclei and core electrons, while the Perdew-Burke-Ernzerhof (PBE) functional^[9] was used to treat electron exchange-correlation interactions. The plane-wave cutoff energy was set to 400 eV, and the k-point mesh was generated using the Gamma-centered method to ensure a sampling density in reciprocal space better than $0.04 \text{ \AA}^{-1}$. During structural optimization, the convergence criteria were set to $0.03 \text{ eV/\AA}$ for atomic forces and 10^{-4} eV for energy. Transition state searches were conducted using the CINEB method^[10], with each transition state confirmed to possess only one imaginary frequency through vibrational frequency analysis.

All surface models were represented using periodic slab models. For instance, the $\text{Fe}_5\text{C}_2(510)$ surface (Figure 1) features a slab model with a thickness of 10 atomic layers, where the bottom 5 layers are fixed, and a vacuum layer of $15 \text{ \AA}$ is set to eliminate interactions between periodic images. The surface calculations employed a supercell of $10.55 \text{ \AA} \times 13.42 \text{ \AA}$, corresponding to a stoichiometric ratio of 58 iron atoms and 24 carbon atoms. In the reaction pathway calculations, the bottom two atomic layers were fixed at their bulk positions, while the top two layers and

adsorbed species were fully relaxed.

The data generation process consists of four main steps: (1) optimization of the clean surface; (2) adsorption structure search; (3) transition state calculation; and (4) vibrational frequency analysis. First, the $\text{Fe}_5\text{C}_2(510)$ clean surface is fully relaxed to obtain a stable surface structure. Subsequently, by systematically varying adsorption sites (such as top, bridge, and hollow sites) and molecular orientations, the most stable adsorption configurations of reaction intermediates are searched. For each reaction step, the CINEB method is employed to connect the initial and final states, identifying the reaction transition state. Finally, vibrational frequency analysis is performed for each stable point (initial state, transition state, final state) to obtain thermodynamic corrections and vibrational properties.

The calculations in this dataset were performed using optimized INCAR parameter settings to ensure a balance between accuracy and efficiency. The plane-wave cutoff energy was set to 400 eV, slightly higher than the ENMAX values of most elements in the POTCAR file, ensuring the completeness of the plane-wave basis set. The electronic self-consistent convergence criterion EDIFF was set to $1 \times 10^{-4} \text{ eV}$ to guarantee the precision of energy calculations^[4,11]. Ionic relaxation employed the conjugate gradient algorithm (IBRION=2), with the force convergence criterion set to $0.03 \text{ eV/\AA}$, ensuring the rationality of the optimized structure^[4,11]. The k-point grid was generated using the Monkhorst-Pack method and set to $2 \times 2 \times 1$. This configuration was optimized for the specific characteristics of surface calculations: the k-point density in the x and y directions (surface plane) was sufficient to describe the periodic electronic structure of the surface, while in the z direction (perpendicular to the surface), only one k-point was necessary due to the presence of a $15 \text{ \AA}$ vacuum layer. The broadening method utilized the Methfessel-Paxton technique (ISMEAR=2) with a parameter SIGMA=0.20 eV, suitable for metallic systems such as Fe_5C_2 . Spin-polarized calculations (ISPIN=2, MAGMOM = 3 for Fe) were enabled to accurately describe the magnetic properties of the iron-based system. Additionally, D3 dispersion correction (IVDW=12) was included to properly account for long-range van der Waals interactions, which is particularly important for calculating molecular adsorption energies.

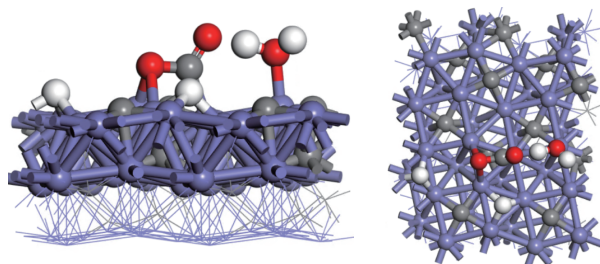


Fig. 1 Top and side views of CO_2 and H_2 adsorption structures on the $\text{Fe}_5\text{C}_2(510)$ surface in the presence of water. Blue: iron atoms, gray: carbon atoms, red: oxygen atoms, white: hydrogen atoms. Thin lines indicate the fixed catalyst substrate during calculations.

1.4 Data sample description

This dataset primarily investigates the reaction processes of C1 molecular catalytic conversion on the Fe_5C_2 polycrystalline surfaces (001, 111, 510), with the corresponding structural counts for each surface being 96, 93 and 472, respectively. Among them, the $\text{Fe}_5\text{C}_2(001)$ surface encompasses three types of reactions: adsorption (e.g., adsorption of species like COH and H_2 at ms/ma sites), dissociation (e.g., decomposition of HCO under H environment), and formation (e.g., generation of products like COH under H environment). The reaction logic on the $\text{Fe}_5\text{C}_2(111)$ surface is similar. Due to its complex stepped structure, the $\text{Fe}_5\text{C}_2(510)$ surface exhibits more diverse reactions: the adsorption phase involves mixed species such as CO_2 and H_2 ; dissociation covers CO/ CO_2 conversion under multiple environments like $2\text{H}_2\text{O}+2\text{H}$ and $\text{H}_2\text{O}+1\text{H}$; and the formation phase can produce low-carbon hydrocarbons like CH_x and CH_4 , as well as intermediates such as HCO and H_2COOH , comprehensively demonstrating the regulatory effects of H_2O coexistence and multi-H environments on reaction pathways. Each subdirectory contains important structural files from VASP calculations, where POSCAR represents the initial structural input, CONTCAR the optimized structure, and OUTCAR includes detailed energy and electronic structure information.

Typical data samples visually illustrate the data encoding rules and reaction information: “Fe001_ads_1H2ma” denotes the adsorption of one H_2 molecule at the ma site on $\text{Fe}_5\text{C}_2(001)$; “Fe001-0.00-Fe56C20” represents the pure surface structure of $\text{Fe}_5\text{C}_2(001)$, presented with 0.00 termination, containing 56 Fe atoms and 20 C atoms, etc. For chemical reactions involving transition states, we use a special symbol (~) to denote them. The field before the ~ symbol represents the reactant, and the field after the ~ symbol represents the reaction product. For example, Fe510_H-O-H-OH-H2O~H-OH-OH-H2O_00 indicates a chemical reaction occurring on the $\text{Fe}_5\text{C}_2(510)$ surface, where the reactant H-O-H-OH-H2O forms the product H-OH-OH-H2O, with 00 representing the initial state structure

and 11 representing the final state structure; Fe510_H-O-H-OH-H2O~H-OH-OH-H2O_01 represents the first structure on the transition state path, and so on. These samples, spanning the entire process from adsorption to dissociation and formation, validate the dataset’s systematic recording of multidimensional information encompassing “surface-environment-species-reaction”, as detailed in Table 2.

1.5 Data quality

To ensure the accuracy and reliability of the computational data, this study rigorously validated the calculation methods. First, the convergence of computational parameters was verified by testing the plane-wave cutoff energy and k-point density. The test results showed that a cutoff energy of 400 eV and a k-point density of $0.04 \text{ \AA}^{-1}$ could achieve total energy convergence within 1 meV/atom. Additionally, the accuracy of the computational method was confirmed by calculating the lattice constants of Fe_5C_2 bulk phase ($a = 11.545 \text{ \AA}$, $b = 4.496 \text{ \AA}$, $c = 4.982 \text{ \AA}$), which closely matched the experimental values ($a = 11.588 \text{ \AA}$, $b = 4.579 \text{ \AA}$, $c = 5.069 \text{ \AA}$). For transition state calculations, each suspected transition state underwent vibrational frequency analysis to ensure the presence of only one imaginary frequency (ranging from -200 to -50 cm^{-1}). For particularly complex reaction pathways, the dimer method was employed for cross-validation to guarantee the reliability of the transition state results.

All adsorption structures and reaction intermediates were optimized using stringent convergence criteria: energy changes less than 10^{-4} eV and atomic forces less than $0.03 \text{ eV/\AA}$. To ensure the attainment of global minima rather than local minima, multiple initial adsorption configurations were tested and compared for each adsorption system. For instance, for the HCOO^* species, various modes such as bidentate adsorption (O atoms interacting with two Fe atoms) and monodentate adsorption (one O atom interacting with Fe) were tested, with the most energetically stable configuration ultimately selected for inclusion in the dataset.

Table 2 Detailed table of dataset structures

Type	Number of structures	Description
Mols	11	Contains different molecules, such as CO_2 , CO, H_2 , H_2O , etc.
Pure surface	17	Presented in the format “Fe[crystal plane index]-[termination parameter]-Fe[number of Fe atoms]C[number of C atoms]” (e.g., Fe001-0.00-Fe56C20), it mainly includes crystal planes such as $\text{Fe}_5\text{C}_2(001)$, $\text{Fe}_5\text{C}_2(10-1)$, $\text{Fe}_5\text{C}_2(110)$, $\text{Fe}_5\text{C}_2(11-1)$, $\text{Fe}_5\text{C}_2(11-3)$, $\text{Fe}_5\text{C}_2(510)$ and $\text{Fe}_5\text{C}_2(511)$
Ads	26	Present in the format “Fe[crystal plane index]_ads/coads_[number of adsorptions][adsorbed species][site]” (e.g., Fe001_ads_1COHms indicates the adsorption of 1 COH specie at the ms site on $\text{Fe}_5\text{C}_2(001)$; Fe510_coads_1CO2_1H2-1 represents the co-adsorption of 1 CO_2 and 1 H_2 structure on $\text{Fe}_5\text{C}_2(510)$)
Reaction	633	Present in the format of “Fe[crystal plane index]_[reactant]~[product]_[state number]” (e.g., Fe510_H-O-H-OH-H2O~H-OH-OH-H2O_00 represents the initial state of “H-O-H-OH-H2O forming H-OH-OH-H2O” on the $\text{Fe}_5\text{C}_2(510)$ surface; Fe510_H-O-H-OH-H2O~H-OH-OH-H2O_11 represents the final state; Fe510_H-O-H-OH-H2O~H-OH-OH-H2O_01 represents the first transition state)

For aqueous systems, the initial arrangement of water molecules considered multiple orientations and positions to ensure the most stable adsorption structure was found. Additionally, frequency calculations were performed to exclude the presence of imaginary frequencies, confirming that all optimized structures reside at minima rather than saddle points on the potential energy surface.

In the domains of machine learning and data mining, the proliferation of high-dimensional data—characterized by a vast number of features or attributes—presents significant challenges that extend beyond mere storage and computational inefficiencies. The phenomenon known as the “curse of dimensionality” exacerbates these issues, as the sparsity and geometric properties of high-dimensional spaces complicate the intuitive understanding of data distribution and intrinsic structure, thereby hindering effective analysis and modeling. Therefore, as shown in Figure 2, we employed principal component analysis (PCA) and t-distributed Stochastic Neighbor Embedding (t-SNE) methods to perform cluster analysis on all our generated structural and energy data. In principal component analysis (PCA), Component 1 and Component 2 represent orthogonal dimensions derived from reducing high-dimensional atomic environment descriptors (such as SOAP vectors), where Component 1 captures the maximum variance in the data and corresponds to the most significant structural patterns, while Component 2 accounts for the second-largest portion of residual variance. PCA highlights differences between systems through linear dimensionality reduction, while t-SNE emphasizes local correlations among configurations (such as the clustering of reaction intermediates in t-SNE space) *via* nonlinear mapping. The PCA similarity plot (Figure 2) visually demonstrates structural similarity through the spatial distribution of points—the closer the points, the more similar the atomic configurations, with different color codes clearly identifying clustering features among systems. The core advantage of the t-SNE visualization lies in preserving local similarity, where the color bar maps formation energy from blue (approximately -800 eV, low-energy stable configurations)

to yellow (approximately -200 eV, high-energy metastable/transition states), directly correlating with structural stability: continuous blue regions correspond to smooth energy evolution during catalyst surface relaxation, while discrete yellow clusters suggest energy barriers or phase transition nodes along the reaction pathway.

1.6 Data usage methods and suggestions

This dataset adopts a hierarchical directory structure for organized access. Each computational subdirectory includes standard VASP files: POSCAR (initial structure), CONTCAR (optimized structure), and OUTCAR (primary output data). Users can select relevant files for analysis based on research objectives. The typical analysis workflow for this dataset includes: (1) Structural parameter extraction: reading bond lengths, bond angles, and other structural information from CONTCAR files; (2) Energy extraction: retrieving energy data from OUTCAR to calculate reaction energies and energy barriers; (3) Electronic structure analysis: analyzing electronic information in OUTCAR to understand the reaction mechanism; (4) Kinetic parameter calculation: combining vibrational frequency data to compute thermodynamic corrections and kinetic constants.

It is recommended to use the following tools for data reading and analysis: (1) Official VASP post-processing tools (such as *vaspkit*, *p4vasp*, etc.) can be used for extracting basic structural parameters and energies; (2) Python materials science libraries (such as *pymatgen*, *ase*, etc.) provide powerful VASP output parsing capabilities, supporting customized data analysis workflows; (3) Visualization software (such as *VESTA*, *OVITO*, etc.) is suitable for structural display and electron density analysis. For beginners, it is advisable to start with the CONTCAR files of typical reaction pathways, visualize the structures of key intermediates and transition states, and establish an intuitive understanding of structure-performance relationships. Advanced users can delve into detailed electronic structure information in the OUTCAR files, such as density of states, charge population, and work function variations.

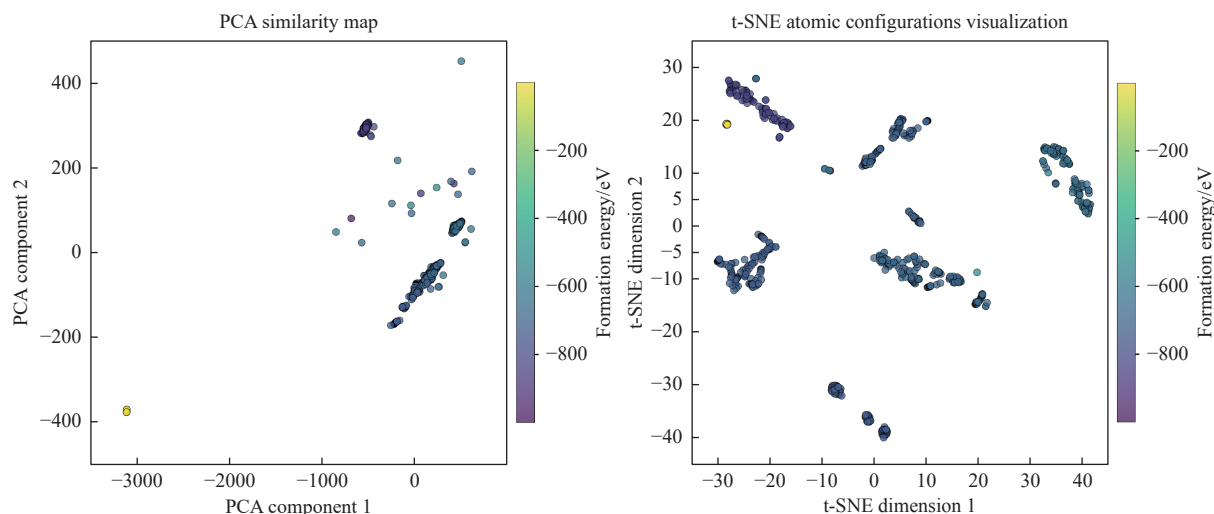


Fig. 2 Cluster analysis of all generated structural and energy data by PCA and t-SNE methods

It should be emphasized that this dataset has certain limitations: Firstly, it employs an idealized periodic slab model, primarily exposing ideal terminations without explicitly including the effects of various defects such as point defects and grain boundaries, which differs from actual industrial Fe-based catalysts (with particle sizes of 10–100 nm and surface defects interacting with supports). Secondly, the calculations are based on 0 K conditions and do not account for industrial reaction parameters such as temperature and pressure. In practical applications, the influence of temperature on dynamic surface structural evolution should be considered. Thirdly, this dataset focuses on the Fe_5C_2 phase and does not include data on other iron carbide phases. In real catalytic processes, phases such as Fe_2C , Fe_3C and Fe_7C_3 may also be involved in addition to Fe_5C_2 . It is recommended that users treat this dataset as foundational reference data and conduct extended analyses tailored to specific research questions. For instance, zero-temperature energy barriers can be converted into apparent activation energies through microkinetic modeling, or structure-activity relationships can be established using machine learning methods to predict the catalytic performance of similar systems.

2 Conclusion

This data paper provides a detailed description of the generation process, content structure, quality control methods, and application value of the computational dataset for catalytic conversion of C1 molecules based on iron-based catalysts. The dataset, produced through systematic density functional theory calculations, investigates the complete reaction pathways of C1 molecules. It includes calculation of adsorption, dissociation, and formation reactions across different crystal surfaces (001, 111, 510) of Fe_5C_2 , including 690 directories and 1961 files. This dataset not only provides high-quality benchmark data for theoretical researchers but also offers theoretical guidance for the design and optimization of industrial catalysts. The data can be directly applied to reaction kinetic analysis, catalytic activity descriptor extraction, and machine learning model training, thereby advancing C1 molecules conversion technologies and supporting China's carbon peaking and carbon neutrality goals.

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.34259.

Declaration of Competing Interest

The authors declare no conflict of interest.

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基于铁基催化剂的 C1 分子催化转化计算数据集

张 建¹, 李超超¹, 路 宽^{2,*}

(1. 山西财经大学 统计学院, 山西 太原 030006;

2. 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: C1 分子(如 CO、CO₂ 等)的催化转化是实现可持续 C1 化学与低碳转型的能源化工核心技术, 其微观反应机理的精准认知需依托系统的理论与实验数据支撑。本研究构建了“基于铁基催化剂的 C1 分子催化转化计算数据集”, 聚焦 Fe₅C₂ 催化剂, 系统整合了不同晶面(如 001、111、510)上 C1 分子吸附、解离与生成反应的多维信息。数据集包含: 多晶面结构数量(Fe₅C₂(001) 构型 96 种、Fe₅C₂(111) 构型 93 种、Fe₅C₂(510) 构型 472 种); 复杂共吸附环境下完整反应路径涉及的物种(COH、H₂ 等吸附态, 2H 条件下 CO 等解离态, 2H 和 H₂O 条件下 CH/CH₃ 等生成态); 按反应类型、晶面、结构参数分类的标准化分级存储体系。该数据集既可作为量子化学计算方法的验证基准, 又能通过揭示晶面与反应机制的耦合效应, 为 C1 分子催化转化中的催化剂设计与反应路径优化提供关键数据支撑。

关键词: Fe₅C₂ 催化剂; C1 分子; 密度泛函理论; 反应机理; 数据集

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文献标识码: A

作者简介:



张建(1989), 博士, 副教授。主要研究方向为统计方法应用, 170214885@qq.com。



路宽(1991), 博士, 副研究员。主要研究方向为计算方法开发及其在化学与材料科学领域的计算模拟应用, lukuan@sxicc.ac.cn。