From "Surface Encapsulation" to "Bulk Penetration" : A Revolutionary Leap in Strong Metal-Support Interaction (SMSI)!

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Abstract

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Full Text

Preamble

From "Surface Encapsulation" to "Bulk Penetration" : A Revolutionary Leap in Strong Metal-Support Interaction (SMSI)!

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Keywords

Strong metal-support interaction; SMSI; Bulk oxygen spillover; Interfacial migration; Bulk-penetration SMSI

1 Introduction

The performance of supported metal catalysts depends on the interface interaction between metal active sites and the support, among which strong metal-support interaction (SMSI) has become a research focus due to its ability to significantly regulate the metal electronic state, adsorption behavior, and catalytic performance [1-3]. The SMSI typically manifests as phenomena such as the formation of special interface structures, reorganization of chemical bonds, and significant electron transfer, exerting a profound impact on the activity, selectivity, and stability of the catalysts [4-6].

In 1978, Tauster et al. first discovered SMSI in the Pt/TiO2 system: after high-temperature reduction, the TiO2 support encapsulates metal particles, leading to a significant reduction in the adsorption capacity of small molecules such as CO [7]. Initially, SMSI research focused on classical reductive SMSI, with core characteristics including the generation of low-valent oxides (e.g., TiOx) from the support induced by high-temperature reduction, which migrate to encapsulate metal particles, accompanied by metal-support electron transfer [8-10]. Subsequently, SMSI research centered around support reducibility (e.g., TiO2, CeO2), metal oxophilicity, and high-temperature reaction conditions, forming the classical cognitive framework of "support species migration-metal surface encapsulation-interfacial electron transfer" (see Fig. 1 [Figure 1: see original paper] A) [11-13]. However, desp ite its advantages, this surface-encapsulation-type SMSI framework has obvious limitations: non-reducible supports (e.g., SiO2, Al2O3) are difficult to form a strict SMSI encapsulation layer, high-temperature conditions easily cause metal sintering, and the encapsulation layer tends to block metal sites.

It is generally believed that one of the basic conditions for the formation of strict strong metalsupport interaction (SMSI) should include the diffusion of support species (i.e., dynamic migration of support clusters or atoms, thereby forming special interface structures and altering the properties of the metal) [14]. Since surface-encapsulation SMSI (SE-SMSI, where support species encapsulate the metal surface through support diffusion) has drawbacks (such as active site shielding and mass transfer hindrance), can bulk-penetration SMSI (BP-SMSI, where support species diffuse into the metal interior through the interface) be designed to address these issues? In April 2026, the joint

team of Tao Zhang, Yanqiang Huang, and Yangang Wang from China published a study in Nature that broke this deadlock [15]: through atomic-resolution transmission electron microscopy and picometer-scale strain analysis, they confirmed that the lattice oxygen (O2-) from TiO2 support can dynamically migrate to the metal Ru bulk phase through the lattice-matched interface (gradually turn the metal into oxide). The "bulk oxygen spillover" process ultimately leads to the formation of a bulk-penetrating structure through the interface, enabling qualitative regulation of the metal electronic state and catalytic performance without surface encapsulation. This discovery shifts the

regulatory core of SMSI from "surface encapsulation architecture" to "bulk penetration architecture"(see Fig. 1 B), providing novel insights for constructing extra SMSI on non-reducible supports and preparing surface-unblocked high-efficiency metal catalysts under mild conditions.

1 Schematic diagrams of the categories of SMSI: (A) surface-encapsulation SMSI (SE-SMSI) and (B) bulkpenetration SMSI (BP-SMSI). SE-SMSI shows support species migration on the catalyst surface, and BP-SMSI shows support species migration in the catalyst bulk.

In this paper, we propose that the key factor of strong metal-support interaction

(SMSI) lies not in whether the support can encapsulat the metal surface, but in whether the species of support undergoes migration and whether it has substantial interfacial electron interaction with metal. The support mass migration (including the migration of oxide clusters, cations, and anions, but excluding electrons and vacancies) is one of the necessary conditions for designing SMSI.

Therefore, under the premise of satisfying mass migration and electronic interaction, for the first time, we divide the SMSI into two main categories: (i) surface-encapsulation SMSI (SE-SMSI) and

(ii) bulk-penetration SMSI (BP-SMSI) (see Fig. 1 for details). For the former, species migration of the support occurs on the catalyst surface; while for the latter, species migration of the support occurs in the catalyst bulk. The BP-SMSI possesses the advantages of the SE-SMSI (electronic structure modulation and performance optimization), while also addressing the challenges faced by traditional SMSI (such as low utilization rate of metal active sites). This paper will systematically review the paradigm shift (or called revolutionary leap) of SMSI from multiple dimensions such as redefinition, mechanism innovation, theoretical breakthroughs, and application upgrading, aiming

to provide a reference for the development of heterogeneous catalytic interface engineering.

2 The core definition, essential connotation and inherent limitations of classical SMSI (namely surface-encapsulation SMSI, SE-SMSI) 2.1 Core definition of classical SMSI (or SE-SMSI) In 1978, Tauster et al. first discovered the SMSI effect in the TiO2-supported Pt catalyst system.

In subsequent work, researchers provided a rigorous definition: under high-temperature reduction conditions (400~600°C, H2), reducible oxide supports (such as TiO2, CeO2) in supported metal catalysts undergo lattice reduction, generating low-valent oxide species (TiO2-x, CeO2-x); these support species migrate to the surface of metal nanoparticles through surface diffusion, forming an ultra-thin coating layer of 1~2 atomic layers (see Fig. 2 [Figure 2: see original paper] A-F and Fig. 1 A) [16~18]; through strong interfacial chemical bonding, large-scale electron transfer, and geometric coating effect, they significantly alter the electronic structure, adsorption properties, and catalytic performances of the metal nanoparticles. Suboxides coating nanoparticles often exhibit amorphous nature and possess dynamic structures under different gas atmospheres. These low-valent oxide overlayers can modify the local electronic structure of the metal surface, and act as Lewis acids, thereby promoting the activation of reactants and enhancing catalytic performances.

Over more than four decades of development, although SMSI has expanded to several subtypes such as oxidation-induced SMSI (O-SMSI) [19, 20], adsorption-induced SMSI (A-SMSI) [21, 22],

covalent MSI (CMSI) [23, 24], and electron MSI (EMSI) [25, 26], the core criteria for determining SMSI in the strict sense have always included three essential elements, none of which can be omitted: (1) Premise of support migration: The solid species (metal cations/low-valent oxide clusters) of the reducible support migrate, rather than merely the transfer of electrons or defects; (2) Characteristic of encapsulation structure: The migrated support species form a partial or complete encapsulation layer on the surface of metal particles, geometrically covering the metal active sites; (3) Essence of performance regulation: Through the synergistic effect of

support migration,

geometrical encapsulation and electron transfer, the adsorption of small molecules such as CO and H2 by the metal is inhibited, and the catalytic activity and selectivity are altered (see Fig. 2 G).

2 Typical cases of classical SMSI (or SE-SMSI): (A-B) Semi-encapsulated Au/TiO2 [16], (C-D) fullencapsulated Au/TiO2 [17], (E-F) full-encapsulated Pt/Fe3O4 [18], (G) structural schematic diagram and core criteria for classical SMSI (or SE-SMSI) with "surface encapsulation architecture" .

2.2 Essential connotation of classical SMSI (or SE-SMSI) In the classical understanding, the "strong" of strong metal support interaction (SMSI), which distinguishes it from ordinary metal-support interactions, is fundamentally underpinned by the surface migration and encapsulation of support species: weak interactions involve only van der Waals forces or electrostatic polarization without material migration; moderate interactions involve only weak electron transfer without long-range diffusion of support atoms; the "strong interaction"

of SMSI is reflected in the profound interaction where support atoms break lattice constraints, migrate across the interface, and reconstruct the metal surface. The "interface fusion at the mass level" is the root cause of electron transfer, structural distortion, and abrupt performance changes.

In summary, the "strong" of SMSI is characterized by four key features: strong interfacial chemical bonding (forming strong covalent bonds such as M–O, M–Ti, M–Ce), large-scale electron transfer (occuring large-scale and condition-dependent electron transfer), deep reconstruction of support and interface (inducing lattice distortion, phase transformation, atomic migration, interfacial alloying,

and defect enrichment), and qualitative modulation of catalytic properties (evidently regulating the catalytic activity, selectivity, sintering resistance, and anti-poisoning capability).

2.3 Inherent limitations of classical SMSI (or SE-SMSI) Firstly, the encapsulation of metals by support oxides often leads to active site shielding, which constitutes a key challenge in classical SMSI. Although the encapsulation of metal nanoparticles by the support can tune catalytic performance, excessive or uneven encapsulation often results in blocking a large number of active metal sites, which may lead to a reduction in overall catalytic activity, especially for reactions requiring direct access to the metal surface. The balance between beneficial electronic modification and detrimental site blocking is delicate and often difficult to precisely control. Secondly, the inherent limitation of classical SMSI lies in the confinement of cognitive boundaries by "surface" and "encapsulation" . Traditional studies suggest that metalsupport interactions occur only at the contact interface between the surface of metal particles and the surface of the support; the bulk phase of the support (below 3~5 atomic layers) acts as an "inert bystander" and does not participate in interfacial mass transfer or reaction regulation. The migration behavior of support species (e.g., oxide clusters and metal cations) is also confined to twodimensional diffusion along the catalyst surface. The metal-support systems without encapsulation and with only electron transfer are excluded from the "strict SMSI" . These cognitive boundaries have created significant bottlenecks in the development of SMSI, limiting a comprehensive understanding of its nature and hindering the rational design of SMSI catalysts.

3 Core findings, microscopic mechanism, and scientific breakthroughs of newtype SMSI (namely bulk-penetration SMSI, BP-SMSI) 3.1 Core findings of new-type SMSI (or BP-SMSI) To address the cognitive limitations of classical SMSI, a team led by Academician Tao Zhang from the Dalian Institute of Chemical Physics, in collaboration with Yanqiang Huang and Yangang Wang [15], focused on the Ru/rutile-TiO2 (r-TiO2) model catalyst (the core system for industrial

hydrogenation and CO oxidation). Using atomic-resolution environmental transmission electron microscopy (ETEM), picometer-precision atomic strain vector analysis, and density functional theory (DFT) calculations, they real-time tracked the migration pathways and structural evolution of oxygen species (support lattice oxygen) at the metal-support interface under reaction conditions (O2 atmosphere, 300~450°C), achieving atomic-level visualization of "bulk oxygen spillover" for the first time (see Fig. 3 [Figure 3: see original paper]) [15]. This study also demonstrated that the migration of support species (anions of oxide) can occur in the bulk phase of catalyst, thereby introducing the new concept in this paper of bulk-penetration SMSI (BP-SMSI) (namely bulk oxygen spillover-type SMSI).

The innovative research on "bulk oxygen spillover [15]" has achieved three disruptive core discoveries, completely rewriting the cognition of mass transfer in SMSI (transition from surface encapsulation to bulk penetration, from metallic cation to non-metallic anion): (1) Oxygen migration pathway (from "surface diffusion" to "bulk interface channel"): In-situ ETEM real-time observation shows that in the Ru/r-TiO2 system, oxygen species do not diffuse two-dimensionally along the TiO2 surface to Ru particles, but instead originate from the TiO2 bulk phase (3~5 atomic layers below the surface), directly migrate directionally into the interior of Ru particles through atomic-level channels at the Ru-TiO2 interface (turning them into RuO2 by the "bottom-up" modle) (see Fig. 3 A-C and Fig. 1 B); Picometer-precision strain analysis confirms that the TiO2 subsurface lattice undergoes reversible local distortion, forming a dynamic oxygen transport channel, and oxygen atoms quickly cross the interface in a "vacancy-mediated" manner.

(2) Migrating species (from "support metal cations" to "lattice oxygen anions"): The migrating species in classical SMSI are support metal cations (Ti3+/Ti4+) or low-valent oxide clusters (TiO2-x); in this study, however, the core migrating species is the lattice oxygen (O2-) of TiO2. Ti cations only serve as the lattice framework, assisting the bulk migration of lattice oxygen through reversible distortion, without undergoing long-range diffusion or surface encapsulation. The finding of nonmetallic anions as migration species has challenged traditional understanding of SMSI . (3) Structural effect (from "support encapsulating metal" to "oxygen permeation reconstructing

metal bulk"): The final result of bulk oxygen spillover is not the support encapsulating the Ru surface, but oxygen atoms embedding into the lattice interstices of Ru particles, forming a Ru-O solid solution, which directly alters the crystal structure, electronic state, and surface adsorption properties of Ru. This structural regulation occurs inside the bulk of Ru particles, rather than only on the surface, and does not require the involvement of a support encapsulation layer.

r-TiO2 (110): (A) at 300 °C , (B) at 450°C 61 s and (C) 450°C 827 s; (D-G) Analysis of oxidation mechanisms of Ru/r-TiO2 by DFT calculation: Structures of (D) interfacial and (E) surface oxidation configurations and their relative interfacial energies per unit area for Ru/r-TiO2, (F) oxygen chemical potential (μo) distribution in different regions of the Ru/RuO2/r-TiO2 system, (G) schematic illustration of the mechanism of interface-controlled bulk oxygen spillover in Ru/r-TiO2 ((1) r-TiO2 surface, (2) r-TiO2 bulk, (3) interfacial RuO2, (4) Ru NP bulk and(5) Ru NP surface); (H) Interior interfacial synergy configuration of Ru/r-TiO2 [16].

3.2 Microscopic mechanism of new-type SMSI (or BP-SMSI) By combining in-situ characterization and DFT calculations, the team proposed an "interface-controlled bulk oxygen transport (i-BOT)" mechanism [15], which consists of three core steps without carrier coating throughout the process: (1) Interface energy level matching triggers oxygen activation (see Fig. 3 D-E): The Fermi levels of Ru and r-TiO2 are aligned, and strong interfacial hybridization causes electrons in the 2p orbitals of TiO2 lattice oxygen to transfer to the d orbitals of Ru. Oxygen atoms are activated and break free from lattice confinement, forming interfacial oxygen

vacancies. Lattice distortion constructs dynamic channels: Migration of activated oxygen atoms induces reversible distortion of the TiO2 subsurface lattice, forming continuous "oxygen vacancy channels". Driven by the chemical potential gradient (see Fig. 3 F), bulk oxygen rapidly diffuses along the channels toward the interface. Oxygen embedding into metal bulk reconstructs the structure: Oxygen atoms crossing the interface embed into the Ru lattice interstices, forming a Ru-O solid solution (Ru undergoes oxidation from the interface outward in a “bottom-up”manner) (see 3 G). Meanwhile, the low migration barrier of oxygen vacancies in TiO2 facilitates oxygen propagation through the “vacancy migration mechanism” within the bulk phase, forming continuous transport channels. Through a 18O isotope tracing experiment, the author directly confirmed that the oxygen in RuO2 originates from the TiO2 bulk lattice, thereby completing a closed-loop verification of the oxygen source. The following conclusions can be drawn: the d-band center of Ru may

downshifts and electron density decreases by bulk oxygen spillover process, ultimately leading to a significant reduction in its CO adsorption capacity and a change in catalytic selectivity.

In addition, this study focuses on comparing two systems: rutile TiO2 (r-TiO2)/Ru and anatase TiO2 (a-TiO2)/Ru (see Fig. 3 H). The former has a low interfacial lattice mismatch and an epitaxial matching structure, while the latter has a high interfacial mismatch with a disordered interfacial structure, providing a direct reference for interfacial regulation of oxygen migration. Key control experiments confirm that for the Ru/a-TiO_2 system, due to high interfacial mismatch and lack of epitaxial matching structure, no bulk oxygen spillover was observed at all; oxygen can only be

weakly adsorbed on the surface, and there is no significant distortion of the Ru structure. These results directly demonstrate that interfacial epitaxial matching is a necessary condition for bulk oxygen spillover, rather than support reduction or surface coating. This discovery significantly expands the scope and boundaries of the SMSI theory, extending the study of catalytic interfaces from “external surface interfaces” to “internal buried interfaces” , and establishing a novel threedimensional synergistic catalytic framework encompassing “surface-interface-bulk phase” .

3.3 Scientific breakthroughs of new-type SMSI (or BP-SMSI)

The core value of the research on interface-controlled bulk oxygen spillover [15] (also called a new-type SMSI with bulk penetration) lies in breaking through the cognitive constraints of classical SMSI and achieving fundamental scientific breakthroughs from the four dimensions as follows:

Definition Breakthrough: SMSI can be formed through oxygen migration without support coating as the core. Strict SMSI no longer requires “support coating on metal” as a necessary condition; oxygen inside the support migrates to the interior of the metal through the interface, causing qualitative changes in the metal structure and electronic state, which meets the new criteria for SMSI: material migration, strong interface interaction, and performance regulation. However, the migrating species can be expanded from “support clusters or cations” to “lattice oxygen anions” , and the migration form can be extended from “surface coating” to “bulk penetration” .

Mechanism Breakthrough: From “surface two-dimensional interaction” to “surface-interfacebulk three-dimensional synergy” . The catalytic effect is no longer limited to the catalyst surface; the support bulk, metal-support interface, and metal bulk form a three-dimensional synergistic system: the support bulk provides the oxygen source, the interface acts as a “selective channel” to regulate oxygen migration, and the metal bulk reconstructs active sites through oxygen insertion. This new mechanism of “bulk participation and interface regulation” completely rewrites the traditional cognition that “catalysis only occurs on the surface” .

Structural Breakthrough: From “support coating metal” to “metal-oxygen-support interface

fusion” . The structural characteristic of SMSI has transformed from the core-shell structure of “support wrapping metal” to a “metal-oxygen-support” continuous interface structure where oxygen atoms bridge the metal and support; oxygen, as an “atomic-level bridge” , realizes continuous coupling of the electronic states of the metal and support, with the coupling depth extending to the bulk of the metal and support, rather than only the surface contact area.

4 Comparative analysis of SE-SMSI and BP-SMSI (revolutionary changes) The core contribution of the 2026 Nature study is to promote SMSI to achieve a revolutionary

leap from “support-encapsulation interfacial interaction” to “bulk oxygen-regulated deep coupling interaction” . The coupling correlation is as follows: interfacial oxygen migration → metal lattice distortion → electronic state change → adsorption property regulation → catalytic performance change, forming a chain-like dynamic correlation, where oxygen acts as a “medium” to achieve real-time coupling between electrons and structure. This study, through atomic-scale in-situ observation, confirms that support lattice oxygen can directionally migrate into the interior of the metal via metal-support interface channels, inducing qualitative changes in the bulk structure and electronic state of the metal without the need for support encapsulation, thus completely subverting the core understanding of classical SMSI that “support encapsulation is the key component” .

Based on this, we have classified SMSI into two main categories: (i) classical surfaceencapsulation SMSI (SE-SMSI) and (ii) new-type bulk-penetration SMSI (BP-SMSI). Meanwhile, we further carry out an essential reconstruction of the definition and connotation of SMSI: SMSI refers to a special interaction in supported metal catalysts under specific conditions (reduction, oxidation, reaction conditions), where the strong chemical bonding (including M-O, M-M bonding modle), large-scale mass migration (including support clusters, cations, lattice oxygen, etc., which can be surface encapsulation or bulk penetration), and surface or bulk reconstruction (accompanied by deep interfacial coupling) occur at the metal-support interface, ultimately leading to qualitative regulation of the metal’ s electronic state, adsorption properties, and catalytic performances. This

classification and redefinition not only break through the cognitive boundaries of SMSI, but also deepen the understanding of the essence of SMSI, guide the precise design of highly efficient catalytic materials, and provide a new theoretical framework and research perspective.

The discovery of "bulk oxygen spillover" -type SMSI marks a paradigm shift in strong metalsupport interaction (SMSI) from "surface encapsulation" to "bulk penetration" . The revolutionary leap from classical surface encapsulation-SMSI (SE-SMSI) to new-type bulk penetration-SMSI (BP-SMSI) can be analyzed comparatively from the following four core dimensions (see Table 1):

Comparison

Classical SMSI (or SE-

Dimension

SMSI) (1978–2025)

Migrating Species

Support metal cations / low-valent oxide clusters (TiO_{2-x}, CeO_{2-x})

New SMSI (or BP-SMSI) (2026, induced by bulk oxygen spillover) Support

lattice

oxygen

anions (O^{2-})

2D diffusion on support

Support bulk → interface

Pathway

surface → metal surface

channel → metal bulk

Support coating on metal

Oxygen embedding into

surface

metal bulk (solid solution

Characteristics

Core Premise

(core-shell

structure)

temperature reduction

Performance

Inhibition of surface small

Regulation

molecule adsorption

supportframework

migration to active oxygen From surface interaction to bulk-interface-bulk

interaction

structure)

Support reducibility + high-

migration

Migration

Structural

Revolutionary Changes

From geometric coating to atomic-level bulk migration

Interface lattice epitaxial

From dependence on support

matching

properties to dependence on

chemical

potential difference Regulation

interface structure

From surface regulation to

electronic state + surface bulk-surface adsorption bifunctionality

synergistic

regulation

5 Conclusions and Prospects This review systematically summarized and analyzed the revolutionary evolution of the strong metal-support interaction (SMSI) field from the classic surface encapsulation type (SE-SMSI) to the new bulk penetration type (BP-SMSI), and draws the following core conclusions:

(1) Subversive breakthrough in definition paradigm: Traditional SMSI (SE-SMSI) cognition regards "support coating the metal surface" as the core criterion for judgment. However, a recent study confirms that support lattice oxygen can directionally migrate to the metal bulk phase through interface channels, inducing qualitative changes in metal structure and

electronic state, and the SMSI effect can be achieved without forming a coating layer (BP-SMSI). We redefines SMSI as "under specific conditions, strong chemical bonding, large-scale mass migration (surface encapsulation or bulk penetration), and surface/bulk reconstruction occur at the metal-support

interface in supported metal catalysts, ultimately achieving qualitative regulation of metal electronic state, adsorption performance, and catalytic performance" . (2) Three-dimensional expansion of the mechanism of action: Classic SE-SMSI is limited to the two-dimensional interaction of "support surface-metal surface", while the new BP-SMSI constructs a three-dimensional synergistic system of "support bulk phase-interface channel-metal bulk phase" .

The support bulk phase serves as an oxygen source reservoir, the interface acts as a selective regulation channel, and the metal bulk phase achieves structural reconstruction through oxygen embedding. Together, they form a chain-like dynamic correlation mechanism of "interface oxygen migration → metal lattice distortion → electronic state change → adsorption performance regulation → catalytic performance optimization", completely rewriting the traditional cognition that "catalysis only occurs on the surface" . (3) Systematic reconstruction of the theoretical framework: This study first classifies SMSI into two major categories: classic surface encapsulation type (SE-SMSI) and new bulk penetration type (BP-SMSI), and conducts an essential comparison from the dimensions of migrating species, migration path, structural characteristics, core premise, and performance regulation. This classification system not only breaks through the dependence of traditional SMSI on support reducibility but also expands the research perspective from "surface interaction" to the threedimensional synergy of "surface-interface-bulk phase" , providing new theoretical guidance for heterogeneous catalytic interface engineering.

In summary, through the review of basic concepts and innovative exploration in the SMSI field, recent study has achieved a revolutionary leap from "surface encapsulation" to "bulk penetration" , opening up new directions for the development of heterogeneous catalytic interface engineering.

Future research can further focus on the precise regulation of interface structure, in situ characterization of dynamic processes, and in-depth construction of theoretical models to promote the application and breakthrough of SMSI technology in extensive industrial catalytic fields.

Acknowledgements

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Classical

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