

中国科学院院长奖申报表

申报类别 中国科学院院长奖

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单位名称 中国科学院山西煤炭化学研究所

学科专业 化学工程与技术

学科专业代 码 081700

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中国科学院人才与人事局制

2026 年 04 月 10 日填

一、基本信息							
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何时何单位何专业获何种学位		2015 年 9 月-2019 年 6 月 郑州大学 工学学士 2019 年 9 月-2022 年 6 月 中国科学院上海高等研究院 工学硕士 2023 年 9 月-至今 中国科学院山西煤炭化学研究所 工学博士					
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	2019 年 9 月-2022 年 6 月	中国科学院大学			工学硕士		
	2023 年 9 月-至今	中国科学院大学			工学博士		
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学年学期		课程名称		学位课	学时	学分	成绩
2024—2025 学年(秋) 第一学期		中国马克思主义与当代		是	36	2.0	91
2025—2026 学年(秋) 第一学期		专题论证		是	40	2.0	92
2025—2026 学年(秋) 第一学期		文献阅读		是	40	2.0	93
2023—2024 学年秋季学期		博士英语		是	64	2.0	92
2023—2024 学年秋季学期		学术道德与学术写作规范		是	20	1.0	95
总学分		9.0		学位课学分		9.0	
论文题目或成果名称		合成气直接制混合醇多功能催化剂的构筑及构效关系研究					
论文（或成果）性质		基础研究					
二、申报人在学期间发表论文、出版专著、专利、获奖情况（请在附件中附有关证明材料）							

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论文名称		全部作者署名排序		发表时间		刊物名称
Hydrogen Spillover-Mediated Spatial Decoupling Process Boosts Syngas Conversion to Higher Oxygenates		Su Li, Zili Ma, Xinyu Zhong, Bo Wu, Jingxuan Guo, Bin Chai, Jianfei Ji, Chengyuan Liu, Jungang Wang, Qiang Wang, Jun Bao, Kegong Fang, Yuhan Sun		2025 年 12 月		Journal of the American Chemical Society
Spatially decoupled Cu/SiO ₂ CoMn catalyst enhances syngas conversion to higher oxygenates		Su Li, Bin Chai, Lei Guo, Yingjun Wang, Kegong Fang		2026 年 1 月		Molecular Catalysis
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三、本人开展的科研工作及取得的成果情况介绍

针对合成气直接制混合醇存在的反应网络复杂、目标产物选择性和 CO 转化率低的科学问题，本人在博士期间致力于构筑空间解耦 Cu 基|CoMn 多功能催化剂体系。在合成气转化反应过程中，多功能催化剂的 Cu 基组元和 CoMn 分别产生 CH_xO^* 和 CH_x^* 中间体，二者之间的协同效应强化 CH_xO^* - CH_x^* 耦合机制，有效地促进了含氧产物的生成。具体研究内容如下所示：

1. 构筑了空间解耦 Cu/SiO₂|CoMn 的模型催化剂，通过精确控制 Cu/SiO₂ 和 CoMn 组分的空间距离和质量比例的匹配方式，实现了优异的催化性能。并揭示了空间解耦 Cu/SiO₂|CoMn 模型催化剂的协同机制，即 Cu⁰ 位点（产生 CH_xO^* ）和 Co⁰-Co₂C 界面（产生 CH_x^* ）不同活性位点在空间上解耦，但是二者的协同作用促进了 CH_xO^* - CH_x^* 耦合。该工作为合成气直接制混合醇催化剂的理性设计提供了新思路。
2. 构筑了不同贵金属改性的 CuM_{0.6}/SiO₂|CoMn (M=Ru、Rh、Pd、Ir、Pt 和 Au) 多功能催化剂，借助贵金属的氢溢流效应，实现了催化剂 CO 转化率和 ROH 选择性的同步提升，其中 Pd 引入具有最高的 ROH 选择性。机理研究证明，贵金属促进了 H₂ 活化和 CH_xO^* 生成，增强了 CH_xO^* - CH_x^* 耦合能力，从而有利于含氧产物的生成。该策略验证了贵金属氢溢流效应在同时提升催化剂活性和 ROH 选择性方面的可行性。
3. 构筑了氢溢流介导空间解耦 Cu_xPd₁/SiO₂|CoMn 多功能催化剂，通过优化 Cu/Pd 最佳摩尔比例和精确控制活性位点的空间排布，成功实现了高 CO 转化率、优异的含氧产物选择性和极低的 C₁ 副产物选择性。基于多种谱学证据与理论计算等，深入研究了 CH_xO^* 中间体的迁移和耦合过程，并且证实了含氧产物经 CH_xO^* - CH_x^* 耦合生成的反应路径。其中，PdCu 单原子合金的氢溢流效应显著促进了 CH_xO^* 中间体迁移至 Co⁰-Co₂C 界面并与表面的 CH_x^* 耦合。该工作提出了合成气制混合醇的新反应机制，验证了 CH_xO^* 迁移并与 CH_x^* 耦合的关键过程，为高效合成气制混合醇催化剂的开发提供了理论依据。

研究成果以第一作者发表在 Journal of the American Chemical Society 和 Molecular Catalysis，如下所示：

1. Li Su, Ma Zili, Zhong Xinyu, Wu Bo, Guo Jingxuan, Chai Bin, Ji Jianfei, Liu Chengyuan, Wang Jungang, Wang Qiang, Bao Jun, Fang Kegong, Sun Yuhua. Hydrogen spillover-mediated spatial decoupling process boosts syngas conversion to higher oxygenates. Journal of the American Chemical Society 2025, 147 (51), 47187-47202.
2. Li Su, Chai Bin, Guo Lei, Wang Yingjun, Fang Kegong. Spatially decoupled Cu/SiO₂|CoMn catalyst enhances syngas conversion to higher oxygenates. Molecular Catalysis 2026, 592, 115745.

四、在政治思想、道德品质、学风等方面自我评价

本人在政治思想上积极拥护中国共产党的领导，遵纪守法，道德品质上追求积极上进，严于律己，注重个人修养，在学风上刻苦努力，锐意进取，勇于探索学科前沿，具备较强的创新意识。

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负责人签名：(公 章)

年 月 日

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类别	博士		主要论文刊物名称（当年 IF）				
专业	化学工程与技术		论文篇数				
联系电话	18838955360		2		20.6	0	
指导教师审核签名							科研工作
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1、Hydrogen spillover-mediated spatial decoupling process boosts syngas conversion to higher oxygenates (A)							
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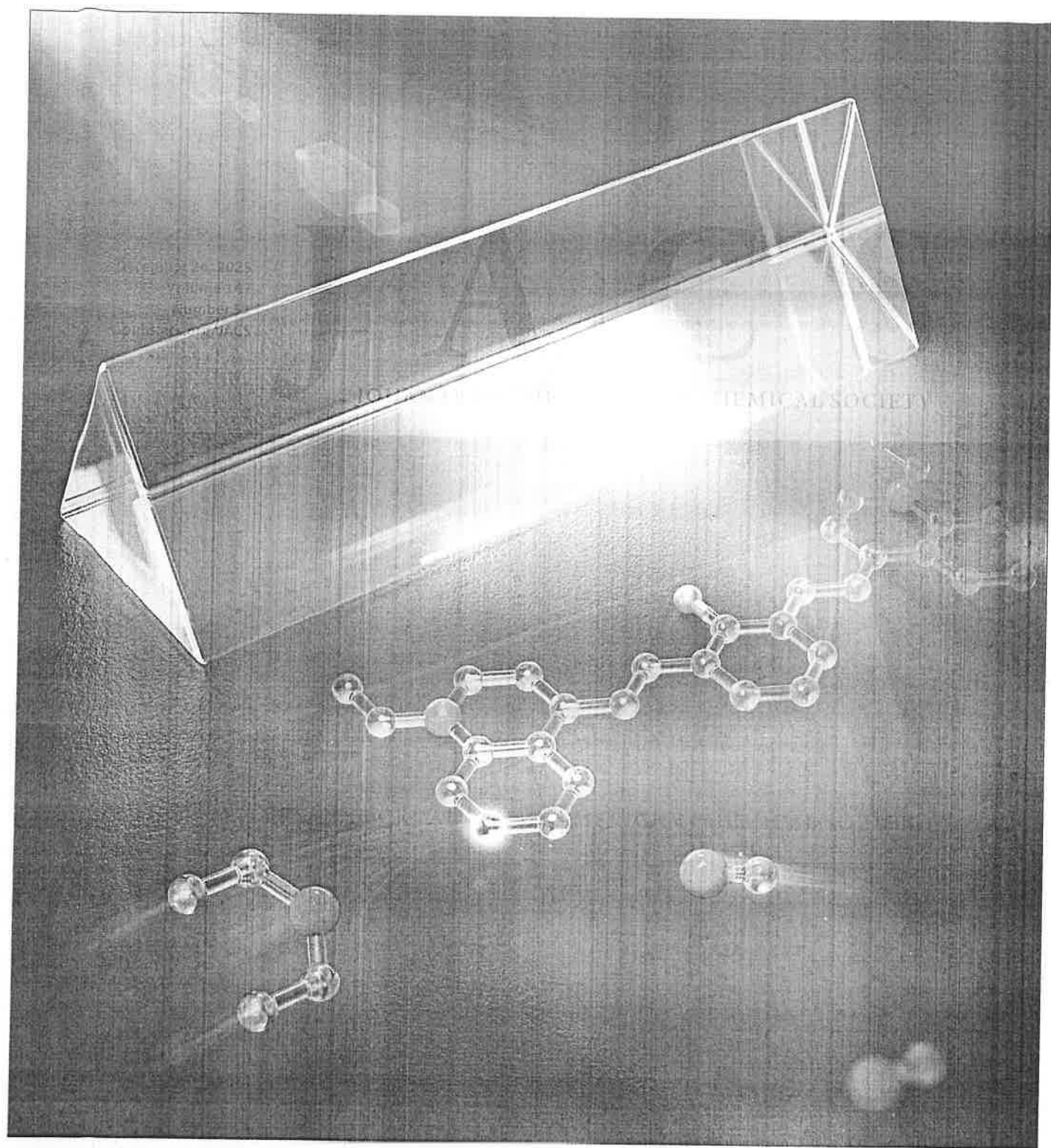
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Hydrogen Spillover-Mediated Spatial Decoupling Process Boosts Syngas Conversion to Higher Oxygenates

Su Li,[†] Zili Ma,[†] Xinyu Zhong,[†] Bo Wu,^{*} Jingxuan Guo, Bin Chai, Jianfei Ji, Chengyuan Liu, Jiangang Wang, Qiang Wang, Jun Bao, Kegong Fang,^{*} and Yuhan Sun^{*}Cite This: *J. Am. Chem. Soc.* 2025, 147, 47187–47202

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ABSTRACT: The direct conversion of syngas to higher oxygenates presents a fundamental challenge in simultaneously achieving high CO conversion, superior oxygenate selectivity, and minimal undesired C₁ byproducts. Here, we develop a series of multifunctional Cu_xPd₁/SiO₂/CoMn catalysts with granule stacking architecture, which overcome the challenge by precisely controlling the spatial arrangement of active sites and the intermediate transport pathway. Systematic optimization reveals a distinct volcano-shaped relationship on Pd loadings, with the Cu₂₈Pd₁/SiO₂/CoMn composite emerging as the optimal candidate. Such a catalyst achieves an exceptional oxygenates molar selectivity of 44.4% (C₂+OH/ROH = 95.4%) while maintaining low C₁ products (6.4% CO₂ and 5.7% CH₄) at considerable 27.3% CO conversion.

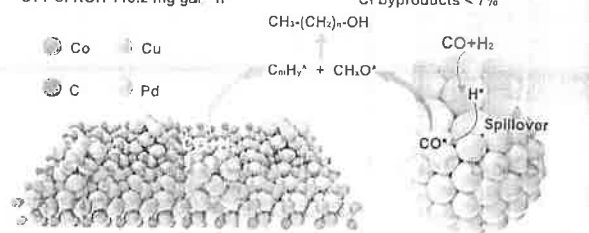
Mechanistic studies reveal that the breakthrough stems from precise control of spatial intimacy of functional components, optimized mass balance between CH_xO* and CH_x*, and isolated Pd atom-mediated hydrogen spillover effects. Based on spectroscopic evidence with theoretical calculations, we propose a synergistic catalytic system wherein PdCu single-atom alloys facilitate H₂ activation and CH_xO* formation through hydrogen spillover, while Co⁰-Co₂C interfaces produce abundant CH_x* species. The synergistic interaction enables the migration of CH_xO* intermediates from single-atom alloy sites to Co⁰-Co₂C interfaces, where they undergo further insertion into CH_x* species, ultimately leading to hydrogenation and formation of higher oxygenates.

High Activity

CO conversion 27.3%

STY of ROH 118.2 mg g⁻¹ h⁻¹

High Selectivity

Oxygenates 44.4%, C₂+OH > 95%C₁ byproducts < 7%

1. INTRODUCTION

Syngas conversion into higher oxygenates (C₂+OH alcohols/aldehydes) offers a sustainable route for fuels and chemicals from coal, biomass, and waste.^{1–5} Among four major catalyst types, Rh-based systems (e.g., Fe–Rh/ZrO₂ and RhFe@SiO₂) offer high ethanol selectivity but are hindered by cost,^{6,7} whereas Mo-based catalysts (e.g., K/Mo₂S and K–FeMo₂C) operate under harsh conditions and generate substantial CO₂ byproducts.^{3,5} Modified methanol catalysts (e.g., K–Cu/ZrO₂ and Cs–Cu/CeO₂) selectively produce isobutanol but suffer from limited chain growth.³ In contrast, modified Fischer–Tropsch catalysts (Co/Fe) stand out by combining high C₂+ oxygenate selectivity,^{1,5} moderate reaction conditions, and efficient chain propagation, positioning them as the most viable candidates for industrial-scale applications. However, the inherently complex reaction network—involving competing and parallel pathways such as H₂ activation, CO dissociation, CO*/CH_xO* insertion, C–C coupling, and water–gas shift reaction—leads to suboptimal activity, low oxygenate selectivity, and undesirable C₁ byproducts.^{3,8,9} To address these challenges, bifunctional catalytic architectures (e.g., Co⁰-Co₂C dual sites) are essential, as they spatially decouple yet

synergistically integrate two critical steps at different active sites.^{10,11} Specifically, we include controlled CO dissociation at metallic cobalt sites and selective CO*/CH_xO* insertion at carbide interfaces. A key thermodynamic hurdle arises from the preferential formation of hydrocarbons,¹² which suppresses CO*/CH_xO* insertion. Consequently, achieving high selectivity of oxygenates requires atomic scale site engineering to precisely modulate the reaction network.

Recent advances in oxygenates synthesis have been driven by two principal catalytic strategies involving dual-site interface engineering^{13–15} and reaction-coupling strategies.^{16,17} Early breakthroughs revealed that closely integrated interfacial architectures such as Cu⁰-Fe₅C₂, Co⁰-Co₂C, and (Fe_xCo_{1-x})₂C could achieve oxygenate selectivity of 30–50%, though these systems continued to struggle with excessive CO₂ forma-

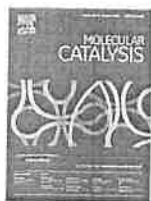
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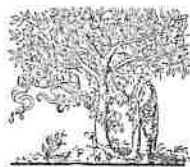
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Spatially decoupled Cu/SiO₂|CoMn catalyst enhances syngas conversion to higher oxygenates

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ABSTRACT

Direct conversion of syngas to higher oxygenates remains a considerable challenge due to the complicated reaction network. Here, we develop a spatially decoupled Cu/SiO₂|CoMn (granule-stacked) multifunctional catalyst with superior catalytic performance, exhibiting 50.5% oxygenates selectivity (C₂₊OH/ROH=95.2%) with low C₁ byproducts formation (10.1% CO₂ and 4.5% CH₄) at 13.2% CO conversion. The spatially decoupled configuration synergistically integrates the distinct active sites between the Cu/SiO₂ and CoMn components by precisely optimizing the proximity and mass ratios, thereby steering the reaction network with high efficiency. Based on spectroscopic results, the synergistic mechanism reveals that the intrinsic role of Cu⁰ sites is responsible for generating CH_xO^{*} species, which then migrate to the Co⁰-Co₂C interfaces, couple with CH_x^{*} species, and thereby boost the oxygenates formation.

1. Introduction

Higher oxygenates are defined as C₂₊ terminal linear α-alcohols and α-aldehydes (C₂₊OH), which are widely applied in fuel additives, detergents, lubricants, and fine chemicals [1,2]. Higher oxygenates synthesis via direct syngas conversion offers a promising alternative route for utilizing non-petroleum carbon resources [3,4], including coal, natural gas, biomass, and solid waste. Modified Fischer-Tropsch (FT) catalysts (e.g., CuFe, CuCo, and CoMn) demonstrate high selectivity and efficient chain propagation capability in syngas conversion to higher oxygenates [1–2,5–6], underscoring collectively significant potential for industrial applications. Typically, modified FT catalysts comprised dual active sites such as Co⁰-Co₂C, wherein the Co⁰ facilitates CO dissociation and C–C coupling while the Co₂C promotes CO insertion. However, the reaction network is inherently complicated, encompassing many consecutive and parallel reactions such as H₂/CO activation, multiple reaction intermediates (CO^{*}, CH_x^{*}, and CH_xO^{*}) formation, C–C coupling, CH_xO^{*}/CO^{*} insertion, and water-gas shift reaction [2,7–8].

To address these challenges, recent advance has focused on dual-site engineering and reaction coupling strategies. Dual-site engineering strategy such as Cu⁰-Fe₅C₂, Cu⁰-Co⁰, (Co_xFe_{1-x})₂C, and Co⁰-Co₂C dual-site

interface [6,9–13], exhibited oxygenates selectivity of 30–50 % while excessive CO₂ byproduct generated. Reaction coupling pathways such as CuZnAlZr|CoMn and FeCo&CuZnAl catalysts [14–15], effectively tuned the reaction networks. This was achieved by synergistically integrating the Cu-based catalyst and the FT catalyst. Although reaction coupling pathways efficiently boost oxygenates formation, the intrinsic role of the Cu sites has been obscured by promoter doping (e.g., Zn, Al, and Zr) and thus requires clarification.

Spatial decoupling refers to the physical separation of different active sites, enabling a synergistic interaction between their respective intermediates, which in turn facilitates the formation of the target product [16]. Herein, we report a granule-stacked Cu/SiO₂|CoMn multifunctional catalyst to probe the intrinsic role of Cu sites. This spatially decoupled configuration integrates distinct active sites between Cu⁰ and Co⁰-Co₂C to steer the reaction network efficiently. By virtue of spatial decoupling, granule-stacked Cu/SiO₂|CoMn catalyst delivers significantly enhanced performance over Cu/SiO₂ and CoMn catalysts. The catalyst demonstrates excellent performance including 50.5 % oxygenates selectivity and low C₁ byproducts formation (10.1 % CO₂ and 4.5 % CH₄) at 13.2 % CO conversion, through optimizing the proximity and precisely controlling the mass ratios of the Cu/SiO₂ and

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