淡江時報 第 1165 期

莊程豪師生論文 躍登《Nature nanotechnology》期刊

學校要聞

【記者麥嘉儀淡水校園報導】物理系主任莊程豪帶領理學院博二生龍友翰和博一生歐茲比，與國際團隊共同攜手合作，設計一種水熱合成法，學術論文〈Ferromagnetic single-atom spin catalyst for boosting water splitting〉（用於促進水分解的鐵磁單原子自旋催化劑）於5月25日刊登於《Nature nanotechnology》自然-奈米技術國際期刊。該期刊影響因子高達44。

這次的跨國研究團隊，包括新加坡國立大學，新加坡科技研究局A*STAR，中國中山大學以及2010年諾貝爾獎得主Kostya S. Novoselov等，國內則有本校及國家同步輻射中心助理研究員盧英睿。莊程豪說明，研究成果展現出鐵磁性單原子材料和其強大鐵電效應，加速海水和純水環境中析氧反應，實現新一代綠色能源中，高穩定性和反應活性研究，此篇文章開創新能源研究領域和未來鐵電應用性。

莊程豪開心地表示：「自然-奈米技術期刊屬於Nature出版社系列下的子期刊，只選定奈米技術和應用的最高等級文章，審查過程非常嚴謹且詳盡，從投稿到接受發表的平均時間，可達到205天之久，平均5年的影響因子係數為42.230，雖比科學《Science》和自然《Nature》期刊的影響數值少一些，但具有更高的學術價值，屬於臺灣奈米界中最夢幻期刊之一。」

他指出，此次重點是設計一種水熱合成法，將可調控磁性鎳原子，摻雜進二維MoS2材料，形成新型單原子自旋催化材料。Ni/MoS2利用一系列原位X光和電子顯微鏡檢測，可證明硫、鎳元素軌域之雜化現象，有效優化自由基中間體的吸附能。當受到外加磁場強化後，其高選擇性自旋電荷轉移，可提升析氧反應（OER）效應達2.88倍。


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nature nanotechnology

Article

https://doi.org/10.1038/s41565-023-01407-1

Ferromagnetic single-atom spin catalyst for boosting water splitting

Received: 21 February 2022

Accepted: 20 April 2023

Published online: 25 May 2023

Check for updates

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Heterogeneous single-atom spin catalysts combined with magnetic fields provide a powerful means for accelerating chemical reactions with enhanced metal utilization and reaction efficiency. However, designing these catalysts remains challenging due to the need for a high density of atomically dispersed active sites with a short-range quantum spin exchange interaction and long-range ferromagnetic ordering. Here, we devised a scalable hydrothermal approach involving an operando acidic environment for synthesizing various single-atom spin catalysts with widely tunable substitutional magnetic atoms (M_1) in a MoS_2 host. Among all the M_1/MoS_2 species, Ni_1/MoS_2 adopts a distorted tetragonal structure that prompts both ferromagnetic coupling to nearby S atoms as well as adjacent Ni_1 sites, resulting in global room-temperature ferromagnetism. Such coupling benefits spin-selective charge transfer in oxygen evolution reactions to produce triplet O_2. Furthermore, a mild magnetic field of ~0.5 T enhances the oxygen evolution reaction magnetocurrent by ~2,880% over Ni_1/MoS_2, leading to excellent activity and stability in both seawater and pure water splitting cells. As supported by operando characterizations and theoretical calculations, a great magnetic-field-enhanced oxygen evolution reaction performance over Ni_1/MoS_2 is attributed to a field-induced spin alignment and spin density optimization over S active sites arising from field-regulated S(*p*)–Ni(*d*) hybridization, which in turn optimizes the adsorption energies for radical intermediates to reduce overall reaction barriers.

Worldwide interest in hydrogen production from water electrolysis with renewable electricity has surged in recent years, since a hydrogen-based economy represents one of the best energy alternatives to the increasing concerns over carbon emissions and climate change[1–4]. However, the bottleneck for efficient hydrogen production via water electrolysis lies in the sluggish kinetics of the oxygen evolution reaction (OER) with the use of scarce precious-metal-based electrocatalysts[4–6]. The sluggish OER kinetics can be attributed to a multiple electron transfer process with the formation of triplet-state molecular oxygen (↑O=O↑) that involves the spin change[7,8]. Despite extensive efforts being devoted to it, the design of efficient and robust non-precious-metal OER spin catalysis with an abundance of desired active sites for the optimization of the

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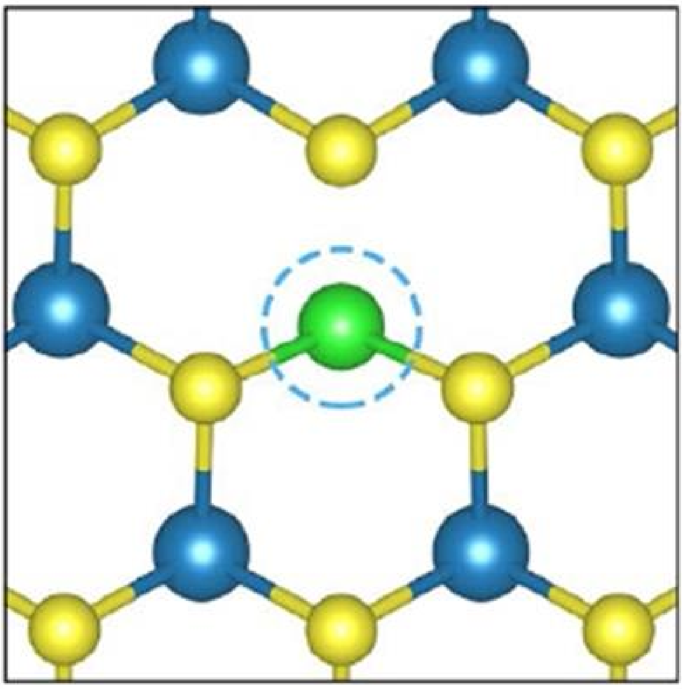

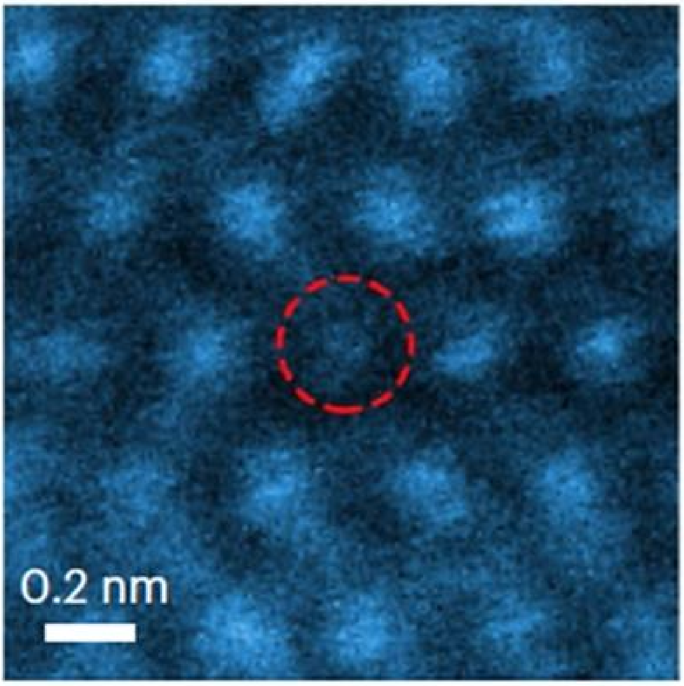
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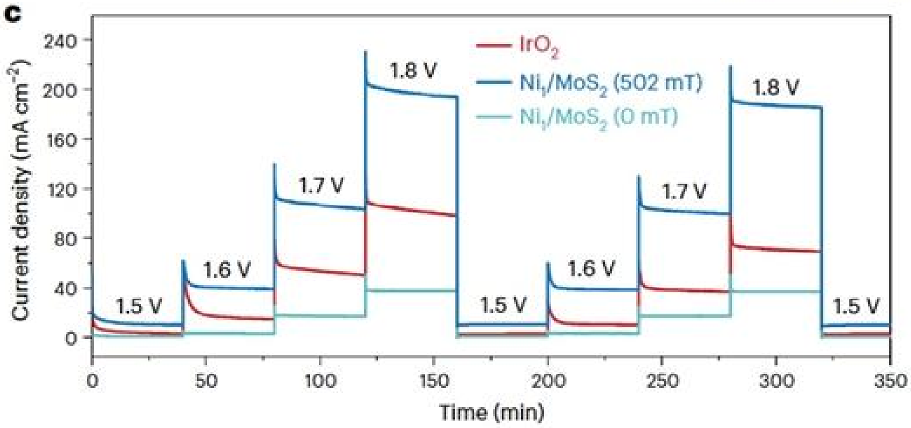
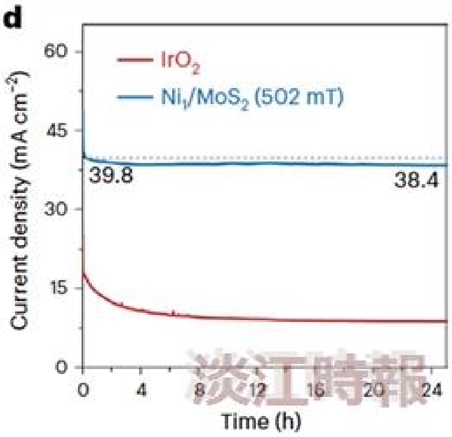

c
IrO$_2$
Ni$_1$/MoS$_2$ (502 mT)
Ni$_1$/MoS$_2$ (0 mT)
1.5 V
1.6 V
1.7 V
1.8 V
1.5 V
1.6 V
1.7 V
1.8 V
1.5 V
Current density (mA cm^{-2})
0
40
80
120
160
200
240
Time (min)
0
50
100
150
200
250
300
350


d
IrO$_2$
Ni$_1$/MoS$_2$ (502 mT)
39.8
38.4
Current density (mA cm^{-2})
0
15
30
45
60
Time (h)
0
4
8
12
16
20
24

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