# 王孝祖2學術論文躍登國際知名期刊

學校要聞

【記者麥嘉儀淡水校園報導】尖端材料科學學程助理教授王孝祖，擔任共同作者之學術論文「A single-atom library for guided monometallic and concentration-complex multimetallic designs 單金屬與不同複合濃度多金屬之單原子合成方法」，獲SCI國際知名期刊《Nature Materials》刊登，影響因子47.7。另一篇擔任共同第一作者之「Bandgap Shrinkage and Charge Transfer in 2D Layered SnS2 Doped with V for Photocatalytic Efficiency Improvement 釩參雜產生二維材料二硫化錫的能隙收縮及電荷轉移來提升光催化效率」，於去年年底刊登《Small》期刊，影響因子15.2，兩篇論文皆在科學界具有非常大的影響力。

本校物理系學、碩士校友王孝祖，為國立清華大學物理博士，師事物理系講座教授彭維鋒及物理系校友、前東華大學校長，中研院院士吳茂昆，與許多國際研究團隊合作。他表示，《Nature Materials》該篇論文合作學者，包括中國科學院學者、美國爾灣大學教授Huolin L. Xin，還有加拿大、美國、臺灣等學者，《Small》該篇則與印度、南非學者合作。

王孝祖說明，剛獲刊登的論文是研究有關單原子的系統，該研究合成利用元素週期表中37種元素，將其單獨合成單金屬單原子，可應用在各種的催化反應，不過，相當不容易合成。此外還進行一系列開拓性研究，由原本的單金屬到成功合成出12種不同元素組成的多金屬單原子材料。「這是一個很大突破，因為我們利用同步輻射技術分析這些單原子系統的價數、鍵長、配位數、配位離子等相關數據，這些數據以後會像教科書一般讓大家據以參考，對於日後研究有非常大的幫助。」

王孝祖指出，另外一篇論文則是探討二維材料在催化上的應用。當二維材料二硫化錫SnS2參雜過渡金屬釩到這個材料裡面，在層與層之間會形成獨特的四面體結構，影響其能隙與電荷轉移機制來提升光催化的效率，並與研發長薛宏中的合作，經過理論計算模擬，證實實驗上所觀察到的結果與理論相符。他表示，這次研究對於未來的綠色能源應用有非常大的突破，可藉此來提升水分解的反應速率，產生大量的氫能源加以利用。

Assistant Professor Hsiao-Tsu Wang of the Bachelor's Program in Advanced Materials Science, is co-author of "A single-atom library for guided monometallic and concentration-complex multimetallic designs, " published on the famous SCI academic journal 《Nature Materials》with an impact

factor of 47.7. Also, he is another co-first author of "Bandgap shrinkage and charge transfer in 2D layered SnS2 doped with V for photocatalytic efficiency improvement ", this paper was published on the SCI journal《Small》at the end of last year, with an impact factor of 15.2. Both papers have a very significant contribution to the scientific community.

Hsiao-Tsu Wang is an alumnus of the Department of Physics at our school. He obtained a Ph.D. in Physics from National Tsinghua University, and was advised by Way-Faung Pong (Chair Professor of the Department of Physics, TKU), and Academician Maw-Kuen Wu (an alumnus of the Department of Physics, TKU and former President of Donghua University). He has cooperated with many international research groups. He said that the co-authors of the paper "Nature Materials", include a scholar of the Chinese Academy of Sciences, Professor Huolin L. Xin at the University of Irvine in the United States, as well as scholars of Canada, United States, and Taiwan, and the "Small" paper cooperated with India and South Africa groups.

2022/10/17


尖端材料科學學士學位學程助理教授王孝祖兩篇學術論文刊登國際知名期刊。（攝影／蕭至芃）

RESEARCH ARTICLE

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# Bandgap Shrinkage and Charge Transfer in 2D Layered $SnS_2$ Doped with V for Photocatalytic Efficiency Improvement

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Effects of electronic and atomic structures of V-doped 2D layered $SnS_2$ are studied using X-ray spectroscopy for the development of photocatalytic/photovoltaic applications. Extended X-ray absorption fine structure measurements at V *K*-edge reveal the presence of V—O and V—S bonds which form the intercalation of tetrahedral O—V—S sites in the van der Waals (vdW) gap of $SnS_2$ layers. X-ray absorption near-edge structure (XANES) reveals not only valence state of V dopant in $SnS_2$ is +4$^+$ but also the charge transfer (CT) from V to ligands, supported by V $L_{2,3}$ resonant inelastic X-ray scattering. These results suggest V doping produces extra interlayer covalent interactions and additional conducting channels, which increase the electronic conductivity and CT. This gives rapid transport of photo-excited electrons and effective carrier separation in layered $SnS_2$. Additionally, valence-band photoemission spectra and S *K*-edge XANES indicate that the density of states near/at valence-band maximum is shifted to lower binding energy in V-doped $SnS_2$ compare to pristine $SnS_2$ and exhibits band gap shrinkage. These findings support first-principles density functional theory calculations of the interstitially tetrahedral O–V–S site intercalated in the vdW gap, highlighting the CT from V to ligands in V-doped $SnS_2$.

## 1. Introduction

The two-dimensional (2D) atomically thin layered metal dichalcogenides have potential in various fields owing to their interesting physical and chemical properties.[1–3] Their rich and tunable anisotropic electronic structures support a remarkable range of functions, which have various optoelectronic applications.[4,5] In the last few years, theoretical and experimental studies of various transition-metal dichalcogenides (TMDs), including $MoS_2$, $MoSe_2$, $TaS_2$, and $WSe_2$, have demonstrated that the anisotropic properties of 2D layered metal dichalcogenides depend strongly on layer thickness, micro-strain, local electronic and crystal structures, the conduction mechanism, and other physical properties.[6,7] Among TMDs, tin disulfide ($SnS_2$) of the IV–VI group has recently emerged as a 2D layered metal sulfide with various applications, such as visible light photocatalysis in $CO_2$ reduction and

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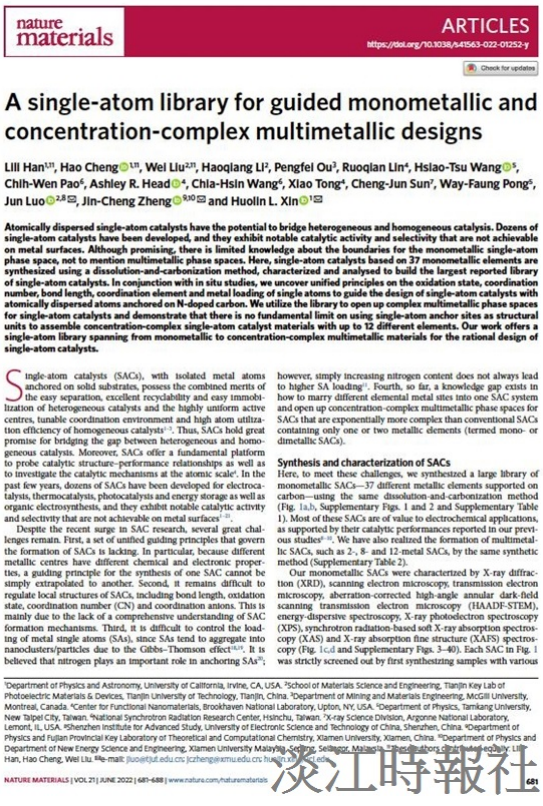
DOI: 10.1002/smll.202105076





尖端材料科學學士學位學程助理教授王孝祖學術論文刊登國際知名期刊。（圖／王孝祖提供）



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https://doi.org/10.1038/s41563-022-01252-y

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# A single-atom library for guided monometallic and concentration-complex multimetallic designs

Lili Han[1,11], Hao Cheng[1,11], Wei Liu[2,11], Haoqiang Li[2], Pengfei Ou[3], Ruoqian Lin[4], Hsiao-Tsu Wang[5], Chih-Wen Pao[6], Ashley R. Head[4], Chia-Hsin Wang[6], Xiao Tong[4], Cheng-Jun Sun[7], Way-Faung Pong[8], Jun Luo[2,8]✉, Jin-Cheng Zheng[9,10]✉ and Huolin L. Xin[1]✉

**Atomically dispersed single-atom catalysts have the potential to bridge heterogeneous and homogeneous catalysis. Dozens of single-atom catalysts have been developed, and they exhibit notable catalytic activity and selectivity that are not achievable on metal surfaces. Although promising, there is limited knowledge about the boundaries for the monometallic single-atom phase space, not to mention multimetallic phase spaces. Here, single-atom catalysts based on 37 monometallic elements are synthesized using a dissolution-and-carbonization method, characterized and analysed to build the largest reported library of single-atom catalysts. In conjunction with in situ studies, we uncover unified principles on the oxidation state, coordination number, bond length, coordination element and metal loading of single atoms to guide the design of single-atom catalysts with atomically dispersed atoms anchored on N-doped carbon. We utilize the library to open up complex multimetallic phase spaces for single-atom catalysts and demonstrate that there is no fundamental limit on using single-atom anchor sites as structural units to assemble concentration-complex single-atom catalyst materials with up to 12 different elements. Our work offers a single-atom library spanning from monometallic to concentration-complex multimetallic materials for the rational design of single-atom catalysts.**

Single-atom catalysts (SACs), with isolated metal atoms anchored on solid substrates, possess the combined merits of the easy separation, excellent recyclability and easy immobilization of heterogeneous catalysts and the highly uniform active centres, tunable coordination environment and high atom utilization efficiency of homogeneous catalysts[1–3]. Thus, SACs hold great promise for bridging the gap between heterogeneous and homogeneous catalysis. Moreover, SACs offer a fundamental platform to probe catalytic structure–performance relationships as well as to investigate the catalytic mechanisms at the atomic scale[4]. In the past few years, dozens of SACs have been developed for electrocatalysis, thermocatalysis, photocatalysis and energy storage as well as organic electrosynthesis, and they exhibit notable catalytic activity and selectivity that are not achievable on metal surfaces[5–10].

Despite the recent surge in SAC research, several great challenges remain. First, a set of unified guiding principles that govern the formation of SACs is lacking. In particular, because different metallic centres have different chemical and electronic properties, a guiding principle for the synthesis of one SAC cannot be simply extrapolated to another. Second, it remains difficult to regulate local structures of SACs, including bond length, oxidation state, coordination number (CN) and coordination anions. This is mainly due to the lack of a comprehensive understanding of SAC formation mechanisms. Third, it is difficult to control the loading of metal single atoms (SAs), since SAs tend to aggregate into nanoclusters/particles due to the Gibbs–Thomson effect[10,11]. It is believed that nitrogen plays an important role in anchoring SAs[12]; however, simply increasing nitrogen content does not always lead to higher SA loading[13]. Fourth, so far, a knowledge gap exists in how to marry different elemental metal sites into one SAC system and open up concentration-complex multimetallic phase spaces for SACs that are exponentially more complex than conventional SACs containing only one or two metallic elements (termed mono- or dimetallic SACs).

## Synthesis and characterization of SACs

Here, to meet these challenges, we synthesized a large library of monometallic SACs—37 different metallic elements supported on carbon—using the same dissolution-and-carbonization method (Fig. 1a,b, Supplementary Figs. 1 and 2 and Supplementary Table 1). Most of these SACs are of value to electrochemical applications, as supported by their catalytic performances reported in our previous studies[9–11]. We have also realized the formation of multimetallic SACs, such as 2-, 8- and 12-metal SACs, by the same synthetic method (Supplementary Table 2).

Our monometallic SACs were characterized by X-ray diffraction (XRD), scanning electron microscopy, transmission electron microscopy, aberration-corrected high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM), energy-dispersive spectroscopy, X-ray photoelectron spectroscopy (XPS), synchrotron radiation-based soft X-ray absorption spectroscopy (XAS) and X-ray absorption fine structure (XAFS) spectroscopy (Fig. 1c,d and Supplementary Figs. 3–40). Each SAC in Fig. 1 was strictly screened out by first synthesizing samples with various

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