Hsiao-Tsu Wang: 2 Papers Published in World Famous Journals

Assistant Professor Hsiao-Tsu Wang, from Bachelor's Program in Advanced Materials Science, has 2 academic papers published in world famous journals as co-author and joint first author respectively : 1) "A single-atom library for guided monometallic and concentration-complex multimetallic designs" in Nature Materials whose impact factor is 47.7, and 2) "Bandgap Shrinkage and Charge Transfer in 2D Layered SnS2 Doped with V for Photocatalytic Efficiency Improvement" in Small with impact factor 15.5.

Asst. Professor Hsiao-Tsu Wang is an alumnus of Department and Graduate Institute of Physics of Tamkang University. He received his Ph.D. degree from National Tsing Hua University. He has been instructed by Chair Professor Way-faung Pong of Department of Physics, Tamkang University and Maw-Kuen Wu, an alumnus of Department of Physics of Tamkang University, former president of National Dong Hwa University, and member of the Institute of Physics at Academia Sinica. Hsiao-Tsu Wang collaborates with numerous international research teams. He stated that the authors of the first paper mentioned above include researchers from Chinese Academy of Sciences, Professor Huolin L. Xin from University of California, Irvine, and others from Canada, The United States, Taiwan and so forth. The second paper stems from the cooperation among researchers from Taiwan, India and South Africa.

Hsiao-Tsu Wang explained that the first paper is a research on single-atom system. The research applies 37 kinds of elements from the periodic table of elements, their synthesis can be used in various catalytic reactions, though was quite difficult. Besides, a series of pioneering research have been conducted and have achieved a breakthrough that will be great help for future studies. The data gained from the research can be referred to like a textbook.

Hsiao-Tsu Wang pointed out that the second paper discusses the application of 2D material in catalytic reactions. He also collaborated with Hung-

Chung Hsueh, Dean of the Office of Research and Development, Tamkang University to theoretically prove the results of the experiment through simulation. He remarked that the research can be applied to improve the reaction rate of water splitting to produce considerable hydrogen, which is of significant breakthrough for the application of clean energy in the future.

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RESEARCH ARTICLE

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

Abhijeet R. Shelke, Hsiao-Tsu Wang, Jau-Wern Chiou, Indrajit Shown, Amr Sabbah, Kuang-Hung Chen, Shu-Ang Teng, I-An Lin, Chi-Cheng Lee, Hung-Chung Hsueh,* Yu-Hui Liang, Chao-Hung Du, Priyanka L. Yadav, Sekhar C. Ray, Shang-Hsien Hsieh, Chih-Wen Pao, Huang-Ming Tsai, Chia-Hao Chen, Kuei-Hsien Chen, Li-Chyong Chen, and Way-Faung Pong**

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 $L_{\alpha,\beta}$ 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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A single-atom library for guided monometallic and concentration-complex multimetallic designs

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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[1–10].

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[9,11]. 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[9–10]. 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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