bimolecular step in CO_2 reduction. Employing an operando XAS technique at **SP 12B1**,[2] Chen's team learned that CuO_x (Cu–O) species could retain their stability during the electrochemical tests (even under potential -0.98 V). According to the XANES spectra (**Fig. 2**), the Cu_4–O_x structure is inferred to be the essential active site for conversion of CO_2 into CO during reduction of CO_2.

In summary, these two works here offer an ideal model of interface design at an atomic level for the reduction of CO_2. The concept of atomically dispersed catalyst is believed to provide an effective and competent supplement to single-atom catalysis, and will provide numerous new opportunities for atomic-level dispersed catalysts to be applied in more complicated catalytic reactions. (Reported by Yan-Gu Lin)

*This report features the work of (1) Xile Hu and his collaborators published in Science **364**, 1091 (2019); (2) Chen Chen and his collaborators published in Nat. Chem. **11**, 222 (2019).*

TLS 20A1 BM – (H-SGM) XAS
SP 12B1 BM – Material X-ray Study

- XANES, EXAFS
- Materials Science, Chemistry, Condensed-matter Physics, Environmental and Earth Science

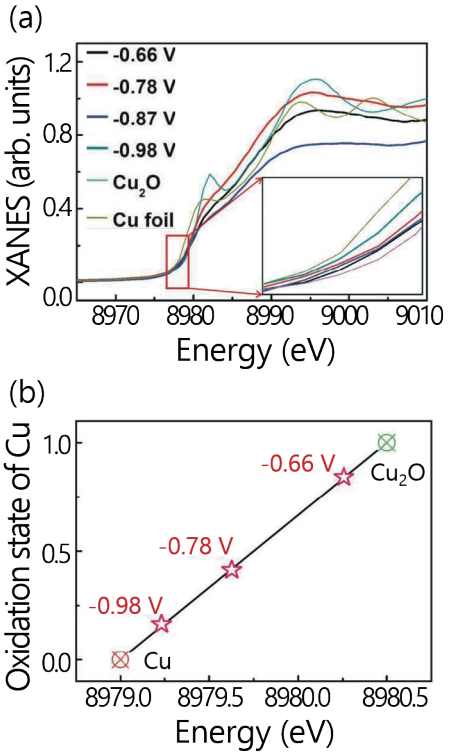

Fig. 2: XAS spectra of catalyst with Cu (0.20 wt%). (a) Cu K-edge XANES spectra *in situ* with various voltages. (b) Oxidation states of Cu with varied voltages from Cu K-edge XANES. [Reproduced from Ref. 2]

References

1. J. Gu, C.-S. Hsu, L. Bai, H. M. Chen, X. Hu, Science **364**, 1091 (2019).
2. J. Jiao, R. Lin, S. Liu, W.-C. Cheong, C. Zhang, Z. Chen, Y. Pan, J. Tang, K. Wu, S.-F. Hung, H. M. Chen, L. Zheng, Q. Lu, X. Yang, B. Xu, H. Xiao, J. Li, D. Wang, Q. Peng, C. Chen, Y. Li, Nat. Chem. **11**, 222 (2019).

Metal Chalcogenide Molecular Accelerates Hydrogen Evolution

An active immobilized single molecular molybdenum disulfide on carbon support was developed.

The production of hydrogen through water splitting using earth-abundant metal catalysts is a promising pathway for converting solar energy into chemical fuels. However, existing approaches for fine stoichiometric control, structural and catalytic modification of materials by appropriate choice of earth abundant elements are either limited or challenging. For example, platinum-based catalytic systems are the most efficient hydrogen evolution reaction (HER) electrocatalysts. However, the low abundance and high cost of precious metals ultimately restricts their large-scale commercial applications. Therefore, the development and pursuit of cheap, noble-metal free electrocatalysts is highly desirable.

Bing-Joe Hwang (National Taiwan University of Science and Technology) and his co-workers recently developed a synthetic approach to fabricate immobilized single molecular molybdenum disulfide (MoS_2) on the surface of carbonized polyacrylonitrile (cPAN), and the electrocatalytic HER of the MoS_2-cPAN composite was performed and benchmarked. Employing X-ray absorption spectroscopy (XAS), X-ray diffraction (XRD), and X-ray photoemission spectra at **TPS 09A**, **TLS 07A1**, and **TLS 24A1**,[1] the team found that the as-prepared material has no metal–metal scattering and it resembles MoS_2 with a molecular state. The local atomic structure of the MoS_2-cPAN catalyst was characterized by XAS of the Mo K-edge, as shown

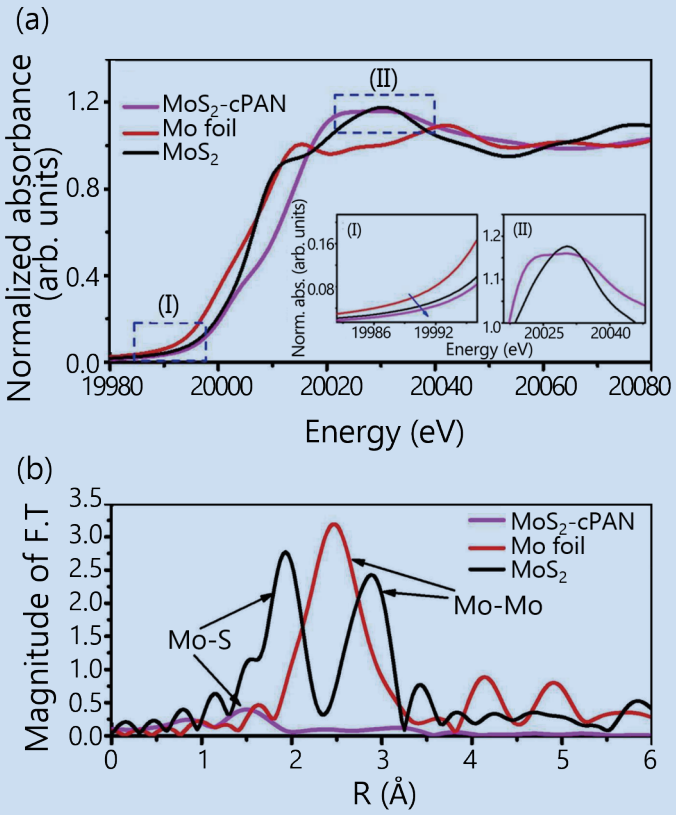

Fig. 1: (a) Mo K-edge XANES spectra of bulk MoS_2, Mo foil, and MoS_2-cPAN; (I) and (II) are enlarged XANES spectra of (a). (b) FTEXAFS spectra at the Mo K-edge of bulk MoS_2, Mo foil, and MoS_2-cPAN. [Reproduced from Ref. 1]

in **Fig. 1**. XPS analyses were also conducted and are depicted in **Fig. 2**. The results imply that the MoS_2 on the surface of carbonized PAN exists in the molecular state and it is suggested that a low coordination number and maximum utilization of the single molecular MoS_2 surface enable MoS_2-cPAN to demonstrate a significantly better electrochemical performance significantly better than that of bulk MoS_2 by two orders of exchange current density and turnover frequency to the hydrogen evolution.

In summary, the single molecular MoS_2 boosts the activity of hydrogen evolution, and this excellent activity is attributed to the low coordination and high vacancy of the 4d orbital of Mo atoms. This work helps to develop highly active single molecular catalysts and explore the fundamental reaction mechanism on the surface of immobilized single molecular catalysts. (Reported by Yan-Gu Lin)

This report features the work of Bing-Joe Hwang and his collaborators published in ACS Nano ***13****, 6720 (2019).*

TPS 09A Temporally Coherent X-ray Diffraction
TLS 07A1 IASW – X-ray Scatteing, EXAFS, XAS
TLS 24A1 BM – (WR-SGM) XPS, UPS

- XANES, EXAFS, XRD, XPS, UPS
- Materials Science, Chemistry, Surface, Interface and Thin-film Chemistry, Condensed-matter Physics

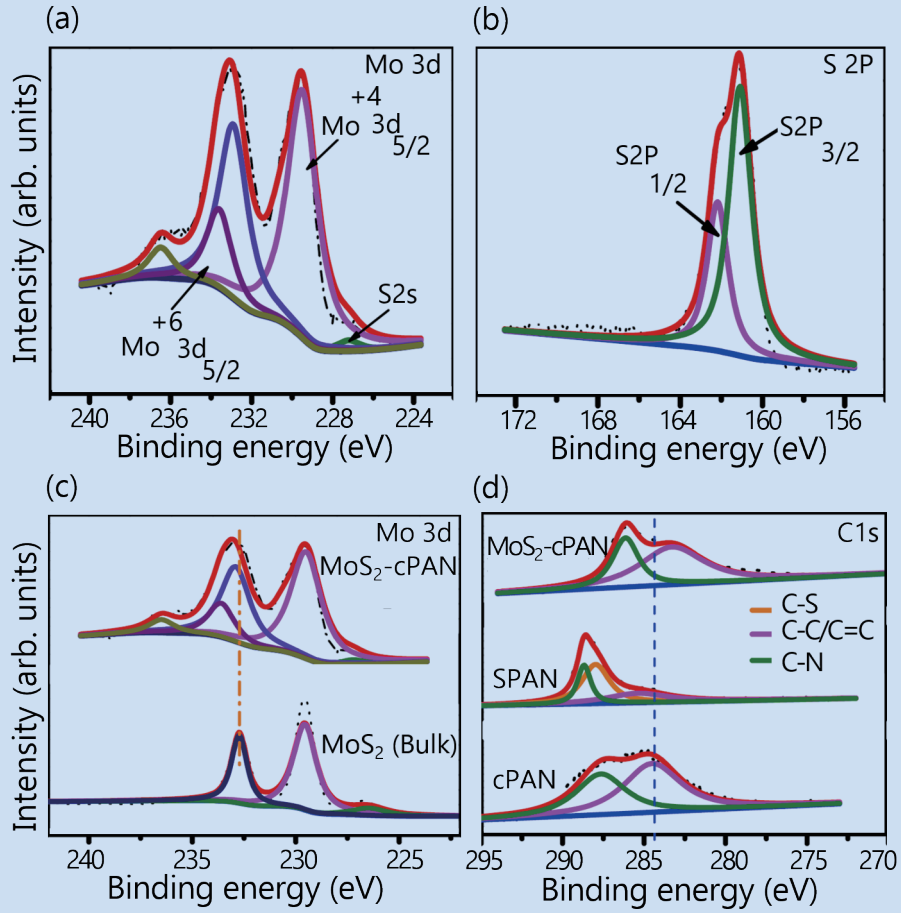

Fig. 2: XPS high-resolution spectra of Mo 3d, S 2p, and C 1s in the energy regions of (a) Mo 3d of MoS_2-cPAN, (b) S 2p of MoS_2-cPAN, (c) Mo 3d of single molecular and bulk MoS_2, and (d) XPS spectra of C 1s for MoS_2-cPAN, SPAN, and cPAN. [Reproduced from Ref. 1]

Reference

1. T. S. Zeleke, M.-C. Tsai, M. A. Weret, C.-J. Huang, M. K. Birhanu, T.-C. Liu, C.-P. Huang, Y.-L. Soo, Y.-W. Yang, W.-N. Su, B.-J. Hwang, ACS Nano **13**, 6720 (2019).