Boosting the Electrocatalytic Activity of Chemically Exfoliated MoS_2 by Surface Functionalization

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The vibrant research area on ultrathin two-dimensional (2D) layered materials has continually shown that the unique and superlative properties firstly observed for graphene find a significant equivalence in other 2D materials as the transition metal dichalcogenides (TMDs). The MoS_2 is an important example which has triggered broad and intense investigations. The 2H-to-1T phase conversion is a semiconductor-to-(semi)metal transition with huge impact on its applications, mainly for electrochemical technologies. The surface functionalization of MoS_2 with a wide variety of species such as metal atoms, organic molecules, metallic nanoparticles, and polymers has been explored as an efficient strategy to modify its intrinsic properties [1,2], for multiple purposes and applications, including phase engineering. In this study, by an experimental-theoretical approach, we show how the chemical functionalization of 1T'-MoS2 with iodoacetic acid molecules improves both the structural stability and the electrocatalytic properties of the metallic nanosheets for the hydrogen evolution reaction (HER) (Figure 1). The presence of -CH_2COOH groups on the MoS_2 surface boosts the electrocatalytic effects for the hydrogen evolution reaction, reducing the charge transfer resistance of the interface and preventing the oxidation and deactivation of the active sites.

References

[1] C. Wang, R. Furlan de Oliveira, K. Jiang, Y. Zhao, N. Turetta, C. Ma, B. Han, H. Zhang, D. Tranca, X. Zhuang, L. Chi, A. Ciesielski and P. Samorì, Nature Communications, 2022, 13, 1–10.

[2] H. Liu, D. Grasseschi, A. Dodda, K. Fujisawa, D. Olson, E. Kahn, F. Zhang, T. Zhang, Y. Lei, R. B. Nogueira Branco, A. L. Elías, R. C. Silva, Y. T. Yeh, C. M. Maroneze, L. Seixas, P. Hopkins, S. Das, C. J. S. de Matos and M. Terrones, Science Advances, 2020, 6 (49).

Figures

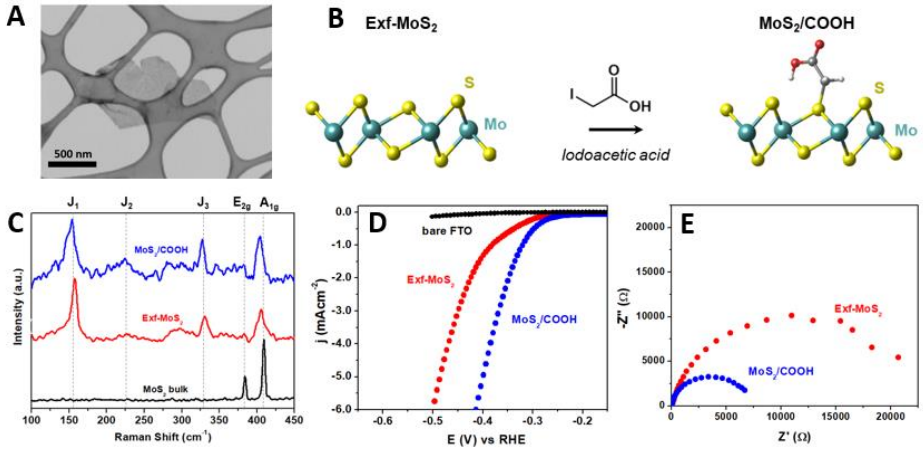

Figure 1: (A) STEM image of chemically exfoliated MoS_2; (B) schematic illustration of the functionalization of MoS_2 nanosheets; (C) Raman spectra of pristine and functionalized MoS_2 and (D-E) electrochemical HER studies of MoS_2 and MoS_2/COOH samples.

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