# Electrochemical Functionalization of 2H-Phase $MoS_2$ nanosheets towards Enhanced Catalytic Applications

**A. Martínez-Jódar***
S. García-Dalí; J.I. Paredes; S. Villar-Rodil; A. Martínez-Alonso; J.M.D. Tascón.
*Instituto de Ciencia y Tecnología del Carbono, INCAR-CSIC, 33011, c/ Francisco Pintado Fe, 26 Oviedo, Spain.*
alberto.mj@incar.csic.es

## Abstract

We describe a novel electrochemical strategy for the surface functionalization of 2H-phase $MoS_2$ nanosheets, which affords the grafting of different molecular groups (e.g., acetic acid groups) derived from organoiodides [1]. Upon cathodic treatment of a pre-expanded $MoS_2$ crystal in an organoiodide containing electrolyte, water-dispersible nanosheets with a derivatization degree of ~0.10 molecular groups per surface sulfur atom were obtained, expanding the scope of covalent molecular functionalization of two-dimensional $MoS_2$, typically restricted to the metastable 1T phase [2]. Functionalization is shown to be driven by the external supply of electrons to the $MoS_2$ nanosheets and to be controlled by the presence of S vacancies in the 2H-$MoS_2$ lattice, where the molecular groups can bind. The functionalized nanosheets were tested as a catalyst for the reduction of nitroarenes and organic dyes with $NaBH_4$, which is relevant in environmental remediation and chemical synthesis [3]. These derivatized 2H-$MoS_2$ nanosheets showed a remarkably enhanced catalytic activity compared to that of non-functionalized 1T- and 2H-phase $MoS_2$ nanosheets as well as non-noble metal catalysts previously reported for this application, and retained a good catalytic activity even at realistic reactant concentrations. The 2H-phase $MoS_2$ catalyst could also be immobilized on a polymeric scaffold in order to facilitate its manipulation and reutilization for several catalytic cycles. Analysis of the reduction kinetics revealed a correlation between the reaction order and the net electric charge of the organic substrates.

## References

[1] S. García-Dalí, J.I. Paredes, S. Villar-Rodil, A. Martínez-Jódar, A. Martínez-Alonso and J. M. D. Tascón. ACS Appl. Mater. Interfaces 2021, 13, 33157-33171.
[2] Paredes, J. I.; Munuera, J. M.; Villar-Rodil, S.; Guardia, L.; Ayán-Varela, M.; Pagán, A.; Aznar-Cervantes, S. D.; Cenis, J. L.; Martínez-Alonso, A.; Tascón, J. M. D. ACS Appl. Mater. Interfaces 2016, 8, 27974−27986.
[3] Tan, C.; Cao, X.; Wu, X.-J.; He, Q.; Yang, J.; Zhang, X.; Chen, J.; Zhao, W.; Han, S.; Nam, G.-H.; Sindoro, M.; Zhang, H. Chem. Rev. 2017, 117, 6225−6331.

## Figures

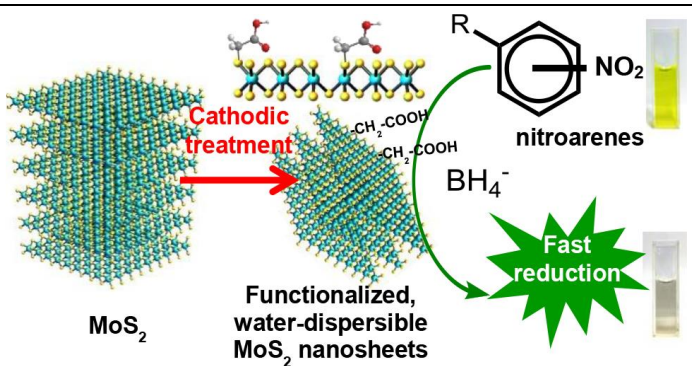


**Figure 1:** Scheme of the electrochemical cathodic strategy used to obtain derivatized 2H-$MoS_2$ dispersions and its application to the reduction reaction of several nitroarenes and organic dyes.