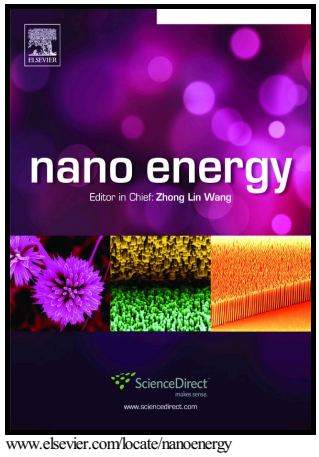

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A photocatalyst of sulphur depleted monolayered molybdenum sulfide nanocrystals for dye degradation and hydrogen evolution reaction

Liangxu Li[a,b], Naihua Miao[c,d], Juntong Huang[a,e], Shaowei Zhang[a,*], Yanqiu Zhu[a], David D. Horsell[a], Philippe Ghosez[d], Zhimei Sun[c], and Dan A. Allwood[b,*]

[a]*College of Engineering, Mathematics and Physical Sciences, University of Exeter, Exeter, EX4 4QL, UK*
[b]*Department of Materials Science and Engineering, University of Sheffield, Sheffield, S1 3JD, UK*
[c]*School of Materials Science and Engineering, Beihang University, Beijing, 100191, China*
[d]*Theoretical Materials Physics, Institut de Physique, Université de Liège, Liège, B-4000, Belgium*
[e]*School of Materials Science and Engineering, Nanchang Hangkong University, Nanchang, 330063, China*

Abstract

Molybdenum disulfide (MoS_2) has a theoretical catalytic activity comparable to Pt but in practice is a poor catalyst in bulk form due to the scarcity of metal edge sites and low electrical conductivity. Recent developments on MoS_2 monolayers (MLs) are more encouraging in developing cheap and efficient catalysts, but the majority metal atoms are on the basal plane are catalytically inactive. The rapid recombination of the electron-hole pairs and electronic band structure of the most stable 2H-MoS_2 MLs are also unsuitable for efficient photocatalysis, especially for solar-driven water splitting. Here, we show that reducing the lateral size and creating sulphur (S) vacancies of MoS_2 MLs not only increases dramatically the density of catalytically active sites, but also adjusts the band structure to become highly suitable for solar-driven catalysis. Besides, this preparation efficiently avoids fast charge recombination associated with MoS_2, improves light harvesting, and gives a newly formed metallic state to transfer electrons for photocatalytic reactions. By way of example, we have demonstrated remarkable photocatalytic degradation of methylene blue (MB) and methylene orange (MO) dye using the S-depleted Mo-S nanocrystals (NCs, 2-25 nm). The NCs are also promising to efficiently generate hydrogen (H_2) from water with sacrificial reagents and solar light irradiation. Our study shows how careful design and modification of materials can result in highly efficient photocatalysts, which give considerable opportunities of the transition metal dichalcogenides (TMDs) beyond just MoS_2 to develop highly efficient and economic catalysts.

Graphical abstract

For applications of photo-chemical (*e.g.* photocatalysis) and photo-physical processes (*e.g.* solar cell), Mo-S monolayers are promising but the efficiencies are low. With careful experimental and theoretical studies, we show how such efficiency (*e.g.* for hydrogen evolution reaction) can be significantly improved through tailoring their electronic structure (*e.g.* band structure, defect levels and suppressed photon recombination) by size reduction and sulphur depletion.