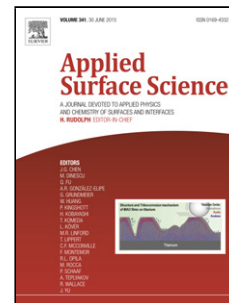


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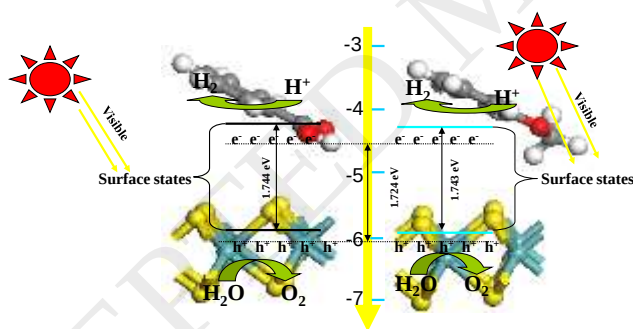
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Graphical abstract



As a fascinating graphene like material with appropriate response for the visible light irradiation, monolayer molybdenum disulfide (MoS₂) is one of the most promising photocatalyst for water splitting. We investigated the functionalization effects of benzoic acid and anisole (C₆H₅COOH and C₆H₅OCH₃) on the photocatalytic performance of monolayer MoS₂. It is found that C₆H₅COOH and C₆H₅OCH₃ both are physically adsorbed on the surface of MoS₂. The functionalization of C₆H₅OCH₃ and C₆H₅COOH on monolayer MoS₂ not only facilitate the separation of photoinduced carriers and improve the adsorption of sunlight, but also make the band positions enough to drive water split into H₂ and O₂. Thus, we propose that the

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