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Role of MoS_2 and WS_2 monolayers on the photocatalytic hydrogen production and pollutant degradation of monoclinic $BiVO_4$: a first-principles study

Francis Opoku[a], Krishna Kuben Govender[b], Cornelia Gertina Catharina Elizabeth van Sittert[c], Penny Poomani Govender[a,*]

[a] Francis Opoku

Department of Applied Chemistry, University of Johannesburg, P. O. Box 17011, Doornfontein Campus, 2028, Johannesburg, South Africa

Email: ofrancis2010@gmail.com

[b] Krishna Kuben Govender
Council for Scientific and Industrial Research, Meraka Institute, Center for High Performance Computing, 15 Lower Hope Road, Rosebank, Cape Town, 7700, South Africa
Email: kgovender3@csir.co.za

[c] Cornelia Gertina Catharina Elizabeth van Sittert
Research Focus Area for Chemical Resource Beneficiation: Laboratory of Applied Molecular Modelling, North-West University, Potchefstroom, 2520, South Africa
Email: cornie.vansittert@nwu.ac.za

*Corresponding author: Penny Poomani Govender
Department of Applied Chemistry, University of Johannesburg, P. O. Box 17011, Doornfontein Campus, 2028, Johannesburg, South Africa
Email: pennyg@uj.ac.za
Tel: +27 11 559 6555

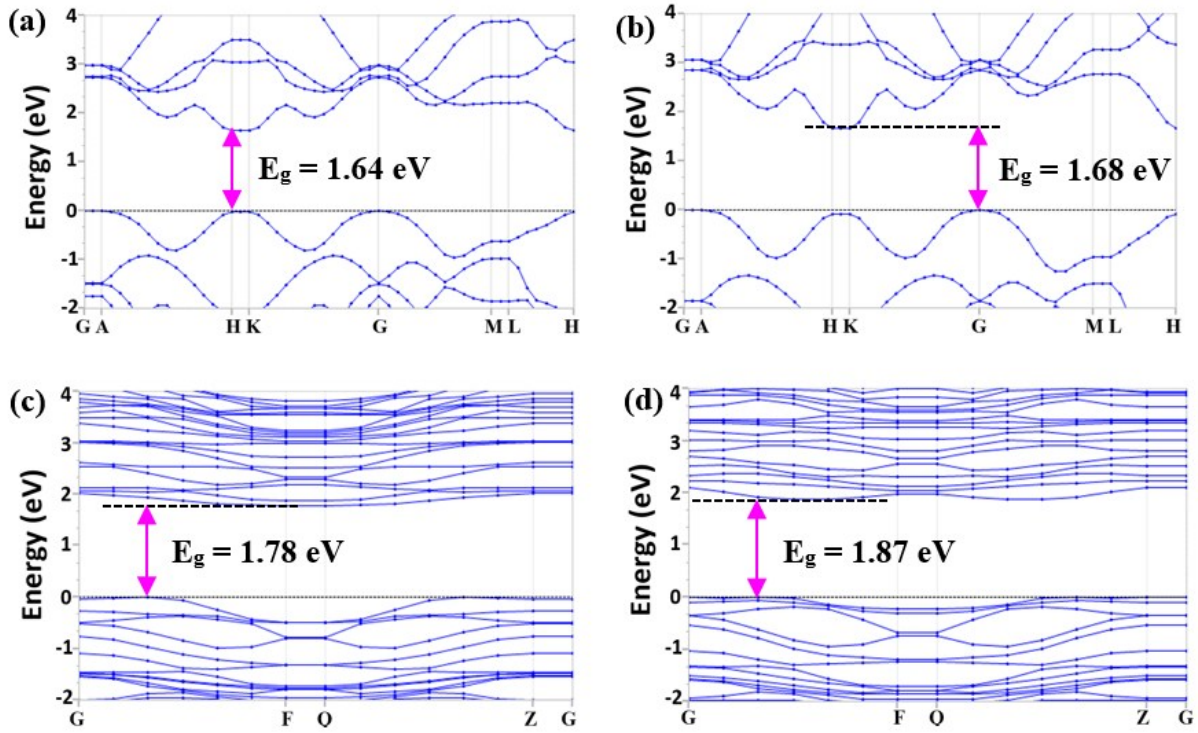

Fig. S1. Calculated unfolded band structure of (a) MoS_2(001), (b) WS_2(001), (c) MoS_2/*m*-$BiVO_4$(010) and (d) WS_2/*m*-$BiVO_4$(010) within the hybrid HSE06 functional. The Fermi level is set to zero as dashed horizontal black line.

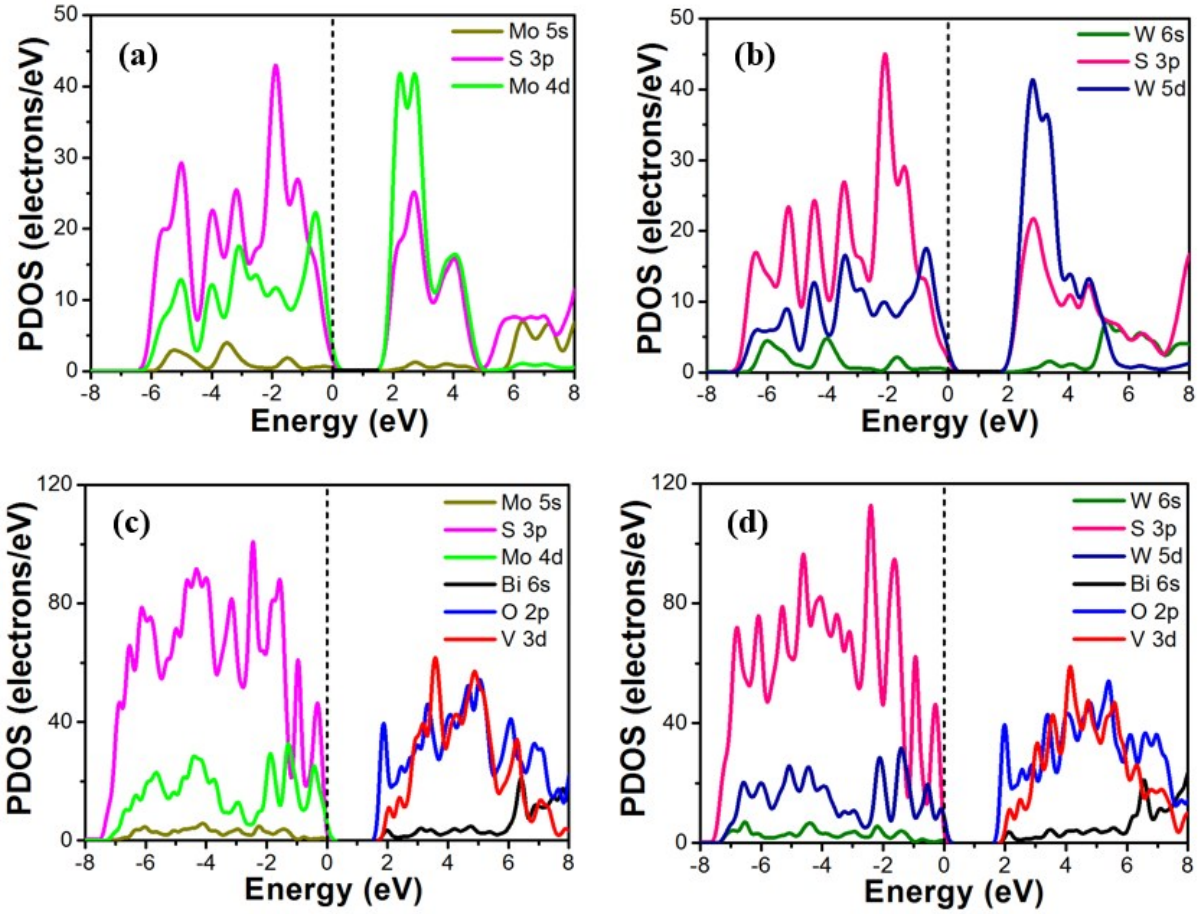

Fig. S2. Calculated PDOS of (a) MoS_2(001), (b) WS_2(001), (c) MoS_2/*m*-$BiVO_4$(010) and (d) WS_2/*m*-$BiVO_4$(010) within the hybrid HSE06 functional. The vertical dashed line is the Fermi level.

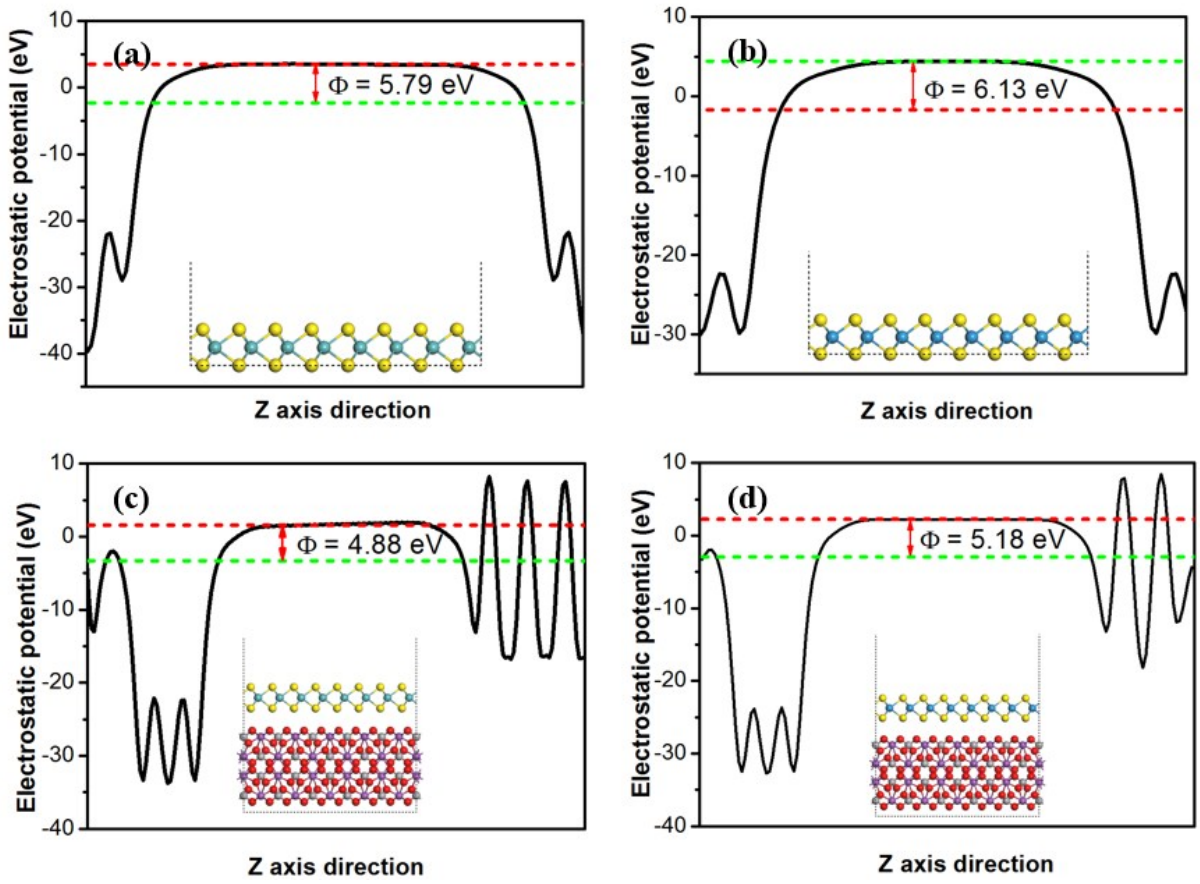

Fig. S3. The work function of the unfolded (a) MoS_2(001), (b) WS_2(001), (c) MoS_2/*m*-$BiVO_4$(010) and (d) WS_2/*m*-$BiVO_4$(010). The red and green dashed lines are the vacuum and Fermi level, respectively.