

Supporting Information

The catalytic activity and mechanism of oxygen reduction reaction on P-doped MoS₂

Xiaoming Zhang^{1,2}, Shaodong Shi¹, Tianwei Gu, Leyi Li¹, Shansheng Yu^{1*}

¹State Key Laboratory of Automotive Simulation and Control, Department of Materials Science, Jilin University, Changchun 130012, China

²Division of Fuel Cell & Battery, Dalian National Laboratory for Clean Energy, Dalian Institution of Chemical Physics, Chinese Academy of Sciences, Dalian 116023, China

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* Corresponding author: Shansheng Yu, E-mail: yuss@jlu.edu.cn

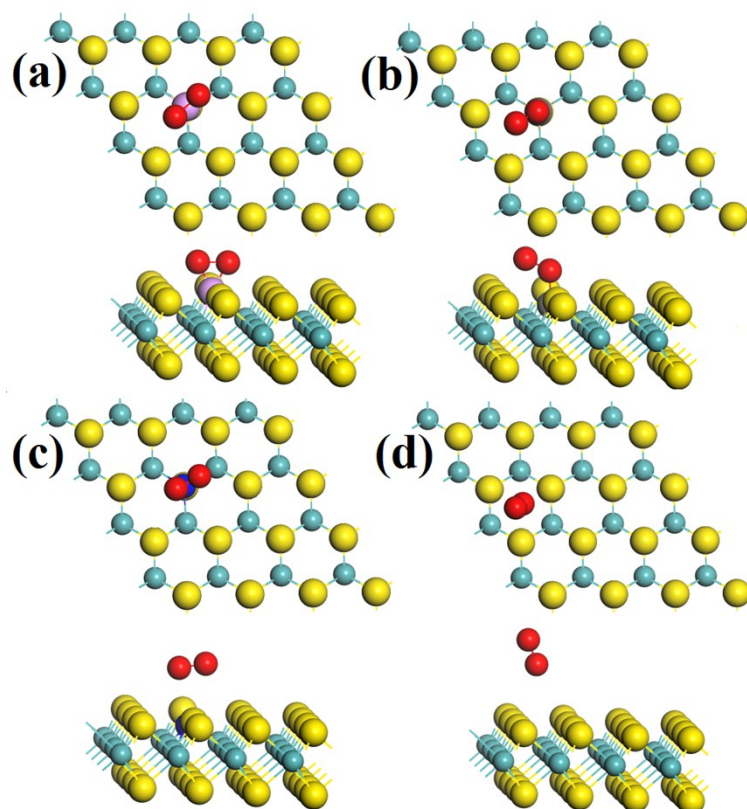


Figure S1 The different kinds of possible adsorption geometries of O_2 .

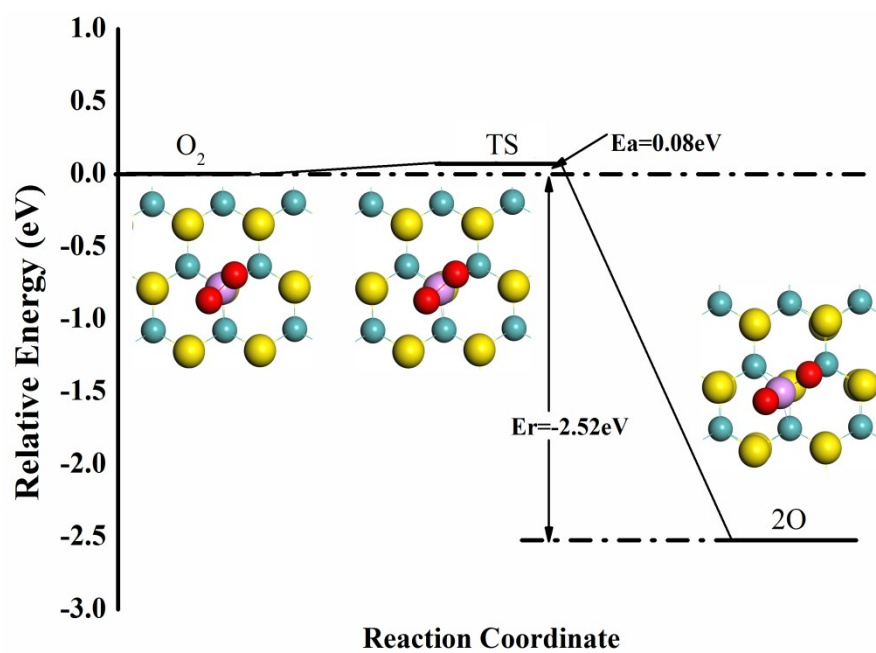


Figure S2 The dissociation step of the oxygen molecule.

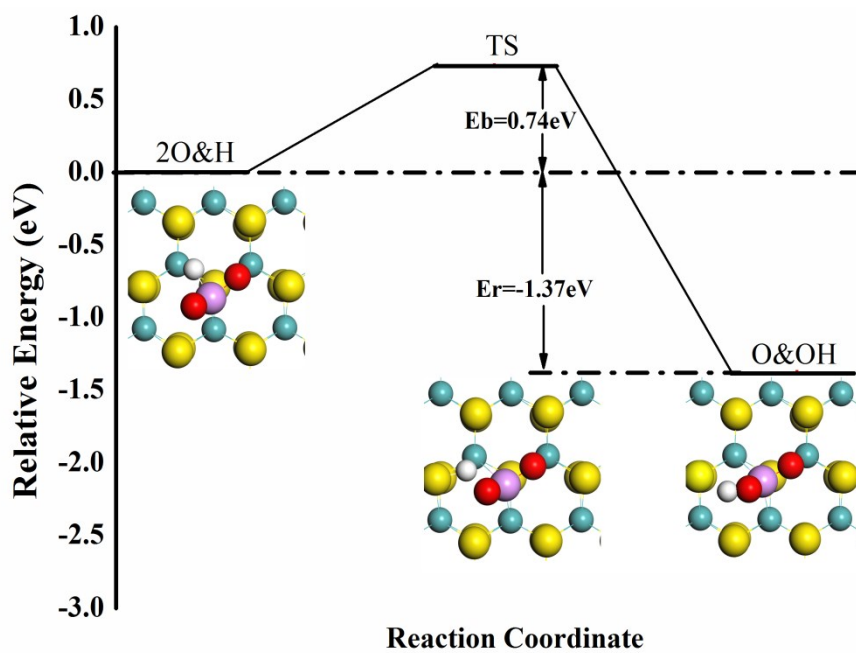


Figure S3 The first hydrogenation step of two atomic O.

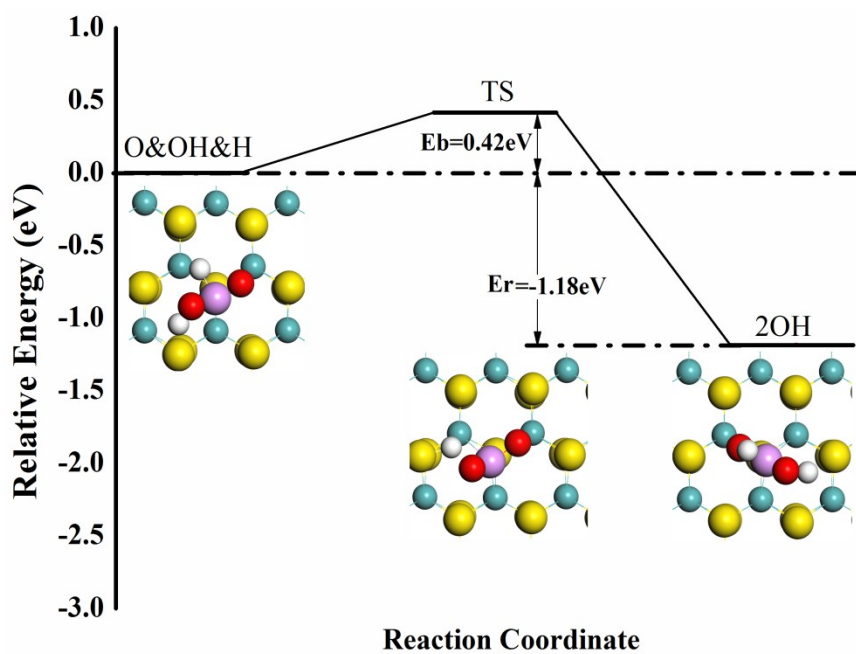


Figure S4 The second hydrogenation step of two atomic O and the formation of two OH species.

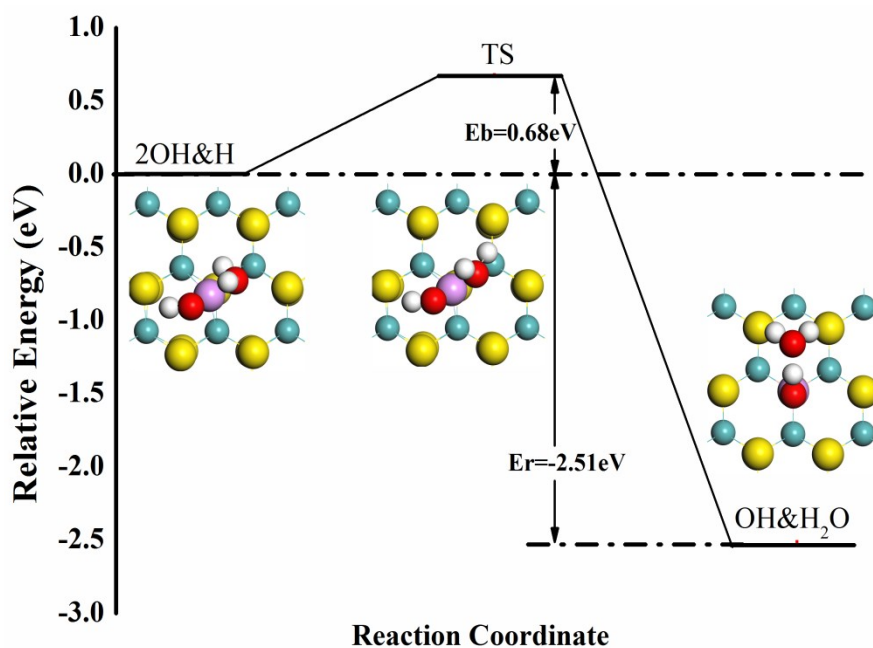


Figure S5 The hydrogenation process of two OH species and the formation of the H₂O from the hydrogenation of the OH, and the release of the H₂O.

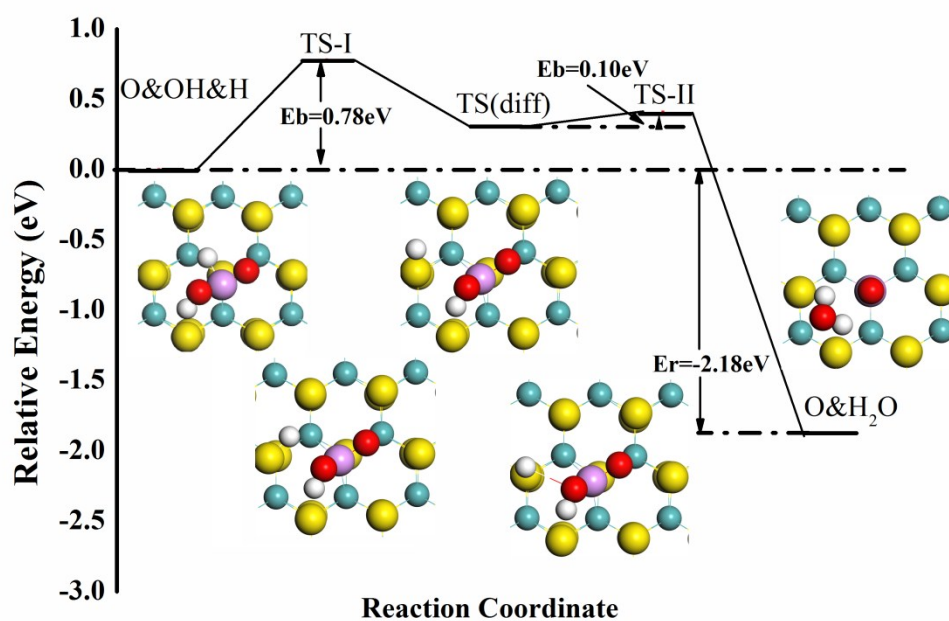


Figure S6 The diffusion of the H atom from the P-Mo bridge site to the S atom near to P and the formation of the H₂O from the hydrogenation of the OH, and the release of the H₂O.

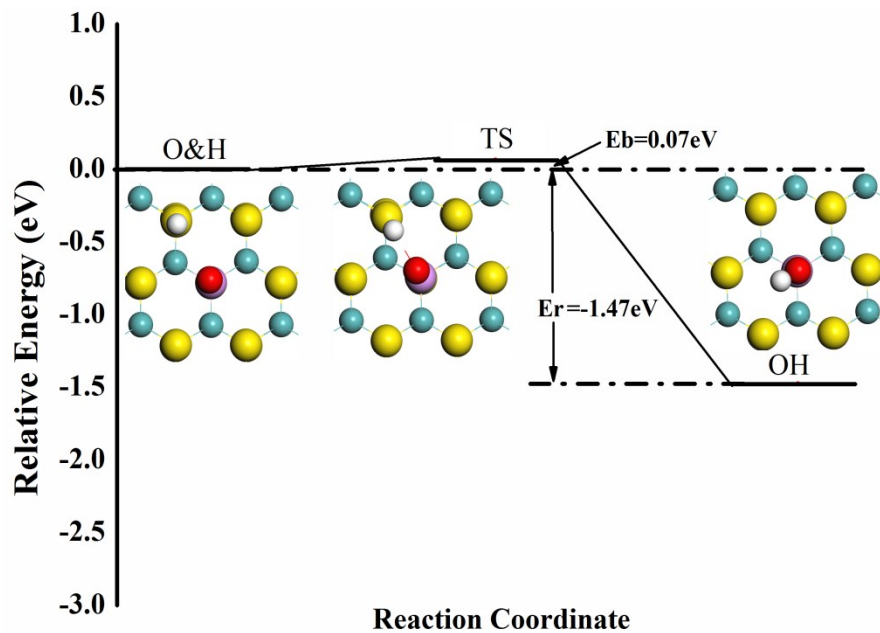


Figure S7 The hydrogenation process of the adsorbed O and the formation of the OH species.

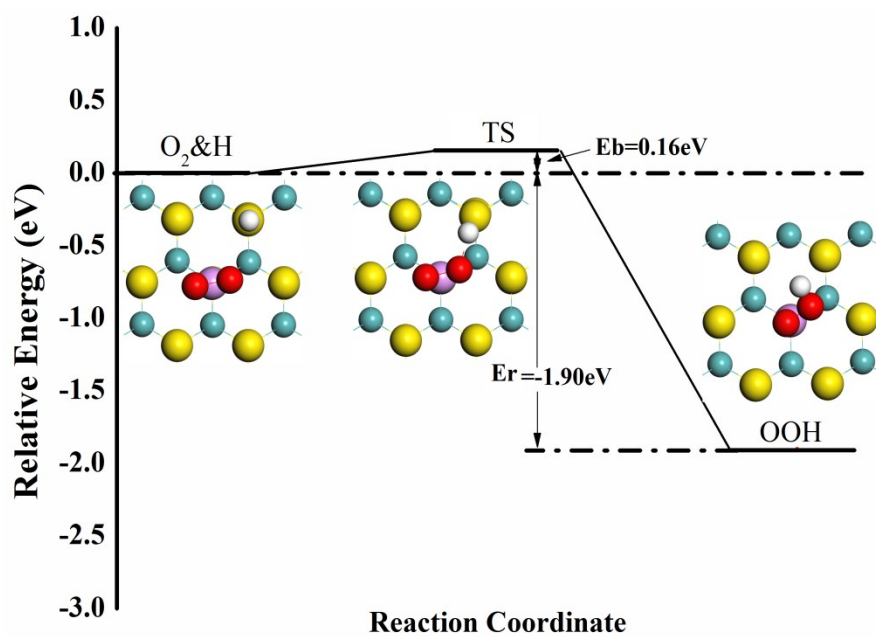


Figure S8 The hydrogenation step of the oxygen molecule and the formation of the OOH species.

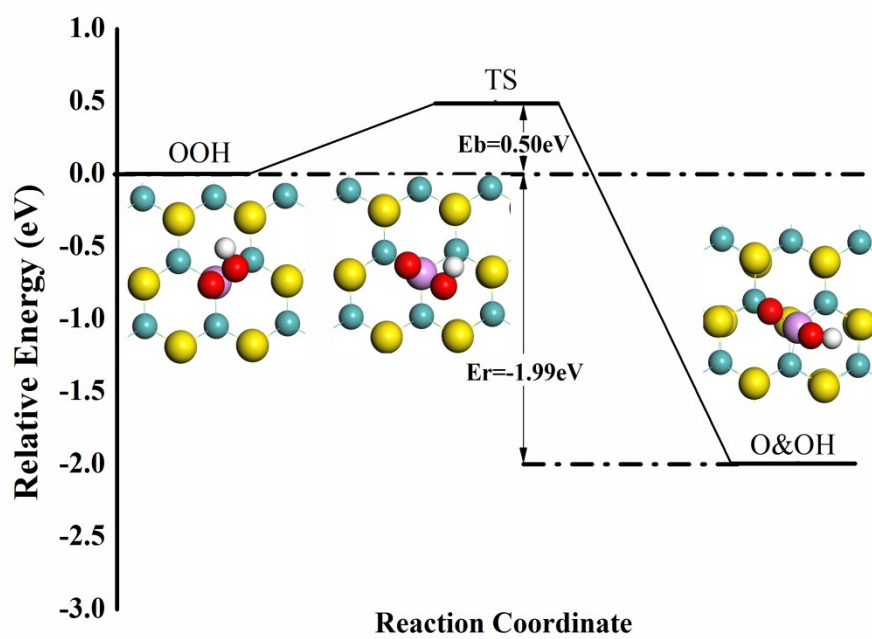


Figure S9 The dissociation of the OOH species into atomic O and OH.