Supporting Information (SI)

Controlling Electronic Properties of MoS_2/Graphene Oxide Heterojunctions for Enhancing Photocatalytic Performance: the Role of Oxygen

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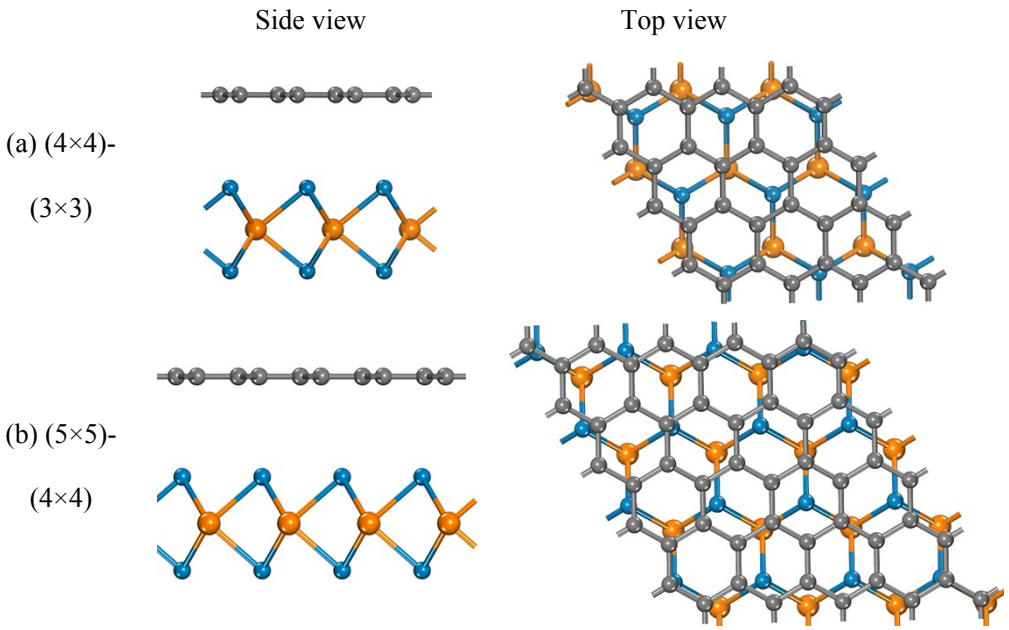


Fig. S1 Side views and top views of two match configurations of MoS_2/GR heterojunctions: (a) match configuration between 3×3 lateral periodicity of 1L MoS_2 sheet and 4×4 lateral periodicity of GR; (b) match configuration between 4×4 lateral periodicity of 1L MoS_2 sheet and 5×5 lateral periodicity of GR.

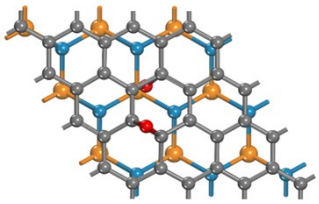
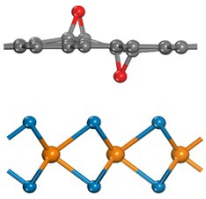
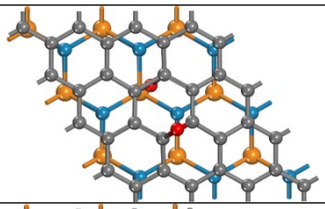
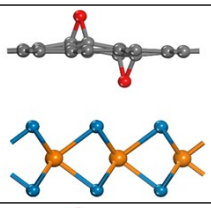
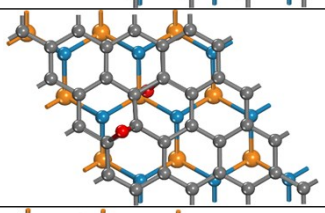
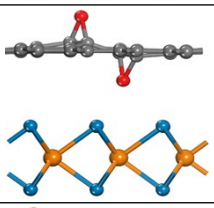
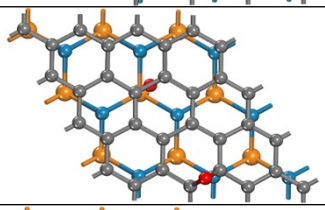
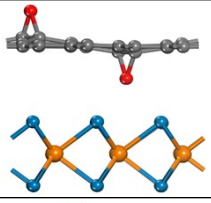
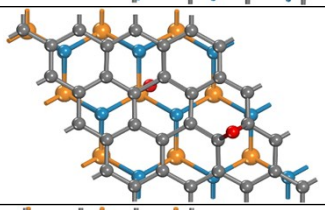
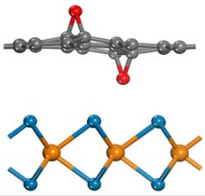
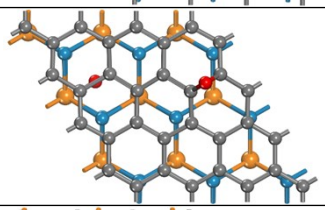
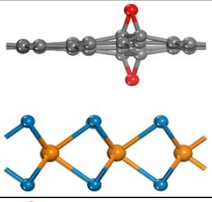
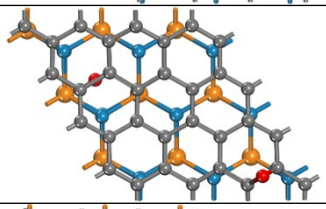
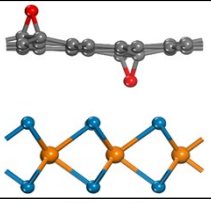
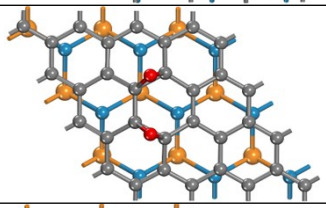
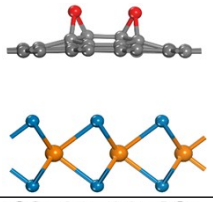
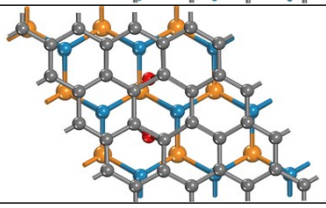
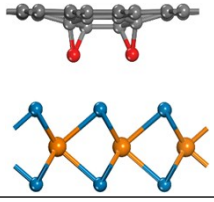
Structure	Top view	Side view	Total energy
MoS_2/GO-A2 **(A2)**			-28289.715
MoS_2/GO-D2			-28288.661
MoS_2/GO-E2			-28289.614
MoS_2/GO-F2			-28289.327
MoS_2/GO-G2			-28289.191
MoS_2/GO-H2			-28289.122
MoS_2/GO-I2			-28289.110
MoS_2/GO-B2 **(B2)**			-28285.583
MoS_2/GO-C2 **(C2)**			-28286.166

Fig. S2 Top views and side views of the optimized MoS_2/GO heterojunctions with two O atoms in interface using GGA-PBE formalism with TS scheme.

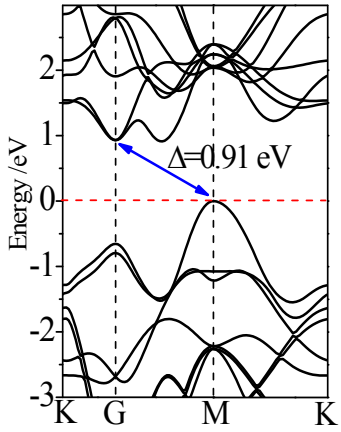
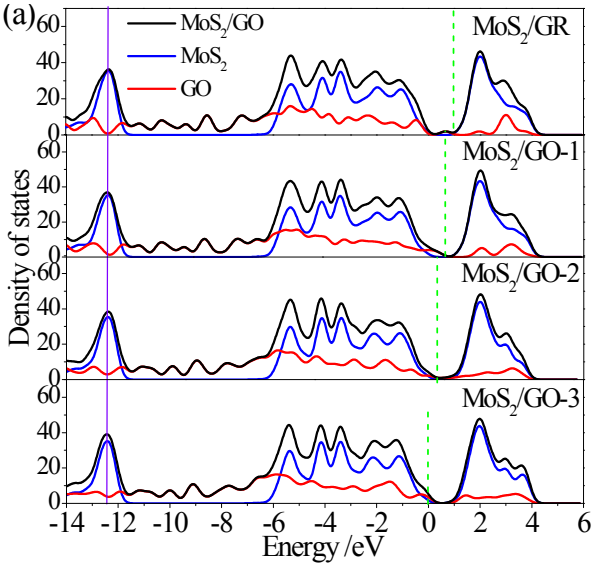


Fig. S3 Energy band structures of bulk MoS_2. The Fermi level is set to zero and marked by red dashed line.



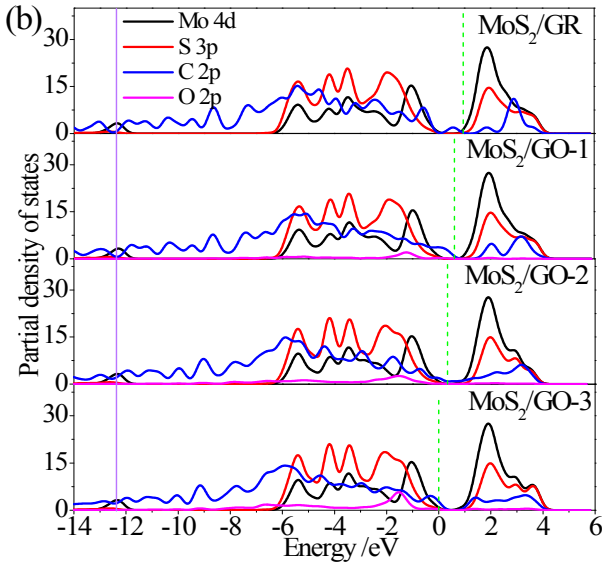


Fig. S4 (a) Density of states of MoS_2/GR and MoS_2/GO heterojunctions, and (b) partial density of states of Mo, S, C and O in the heterojunctions with different O concentrations. The peak of C 2p state at -12.4 eV is taken as the reference point to calibrate the energy levels near the Fermi levels. The Fermi levels are marked by green dashed lines.

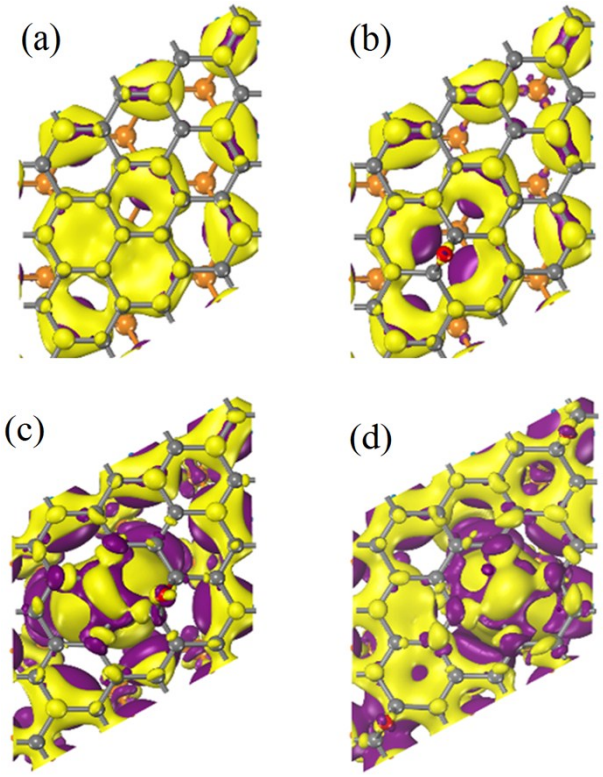


Fig. S5 Side views of the 3D charge density differences of (a) MoS_2/GR, (b) MoS_2/GO-1, (c) MoS_2/GO-2, and (d) MoS_2/GO-3 heterojunctions.