Supplementary Information

Novel heterostructures by stacking layered molybdenum disulfides and nitrides for solar energy conversion

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\textbf{Fig. S1} The band structures of monolayers and bilayer heterostructures calculated with HSE06: (a) g-AlN, (b) g-GaN, (c) MoS\textsubscript{2}/g-AlN, (d) MoS\textsubscript{2}/g-GaN.

\textbf{Fig. S2} The electronic structures of (a) monolayer and (b) bilayer MoS\textsubscript{2}, calculated with HSE06.