

Supporting Information for

Janus Structures of Transition Metal Dichalcogenides as the Heterojunction Photocatalysts for Water Splitting

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Table S1. Band gaps (eV) of pristine MoX₂ and Janus MoXY structures calculated by HSE06 functional with and without considering the spin-orbital coupling effects.

	MoO ₂	MoS ₂	MoSe ₂	MoTe ₂		
HSE06	1.48	2.09	1.86	1.49		
HSE06+SOC	1.47	2.01	1.76	1.37		

	MoOS	MoOSe	MoOTe	MoSSe	MoSTe	MoSeTe
HSE06	1.55	1.32	0.66	1.98	1.53	1.70
HSE06+SOC	1.53	1.30	0.61	1.90	1.51	1.60