Electronic Supplementary Information

High efficient photocatalytic water splitting and large piezoelectric properties of 2D Janus group-III chalcogenides

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GaInSSe		GaInSTe		GaInSeTe		InGaSSe		InGaSTe		InGaSeTe	
S	0.8121	S	0.8299	Te	0.4793	Se	0.6624	Те	0.4778	Se	0.6918
In	-0.8688	In	-0.8569	In	-0.5447	In	-0.6922	In	-0.5388	In	-0.7069
Ga	-0.6024	Ga	-0.4042	Ga	-0.6016	Ga	-0.7862	Ga	-0.7598	Ga	-0.4203
Se	0.6590	Te	0.4311	Se	0.6669	S	0.8161	S	0.8208	Те	0.4355

Table S1. The Bader charge transfer of MM'XX' monolayers.



Fig. S1 Band structures of Janus M2XX' calculated by HSE06 method.



Fig. S2 Band structures of Janus MX calculated by HSE06 method.



Fig. S3 The partial charge density of VBM and CBM for Janus MM'XX' monolayers.