Supplementary Materials

Novel Janus XGa–PbP (X = S, Se) monolayers: excellent photocatalysts for overall water splitting

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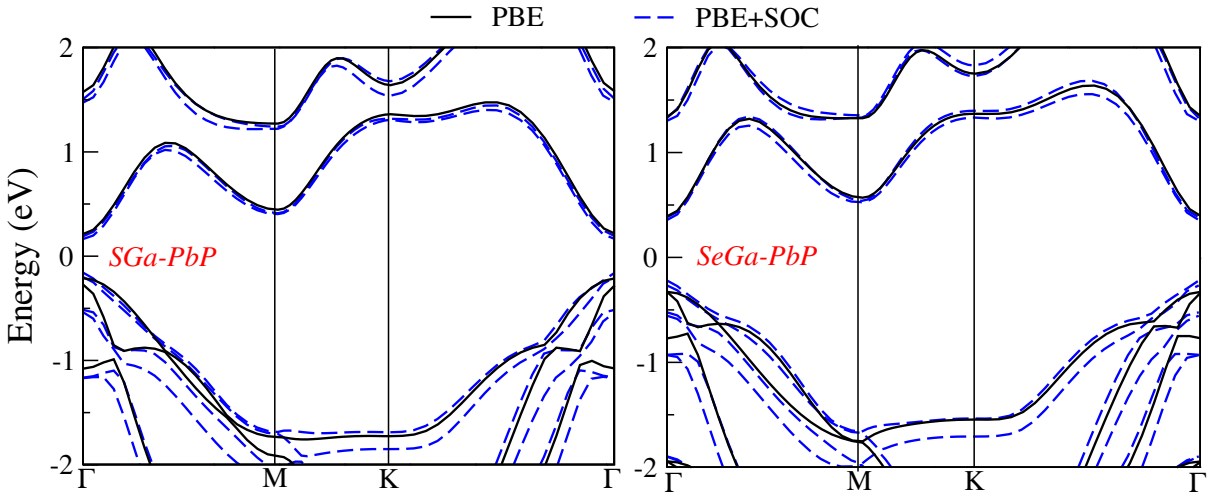

Figure S1: Band structures of the SGa-PbP and SeGa-PbP monolayers calculated using PBE and PBE+SOC

Table S1: Band gaps (E_g) of SGa–PbP and SeGa–PbP monolayers from PBE and PBE+SOC calculations, with their differences ΔE_g .

System	E_g^{PBE}	$E_g^{PBE+SOC}$	ΔE_g
SGa-PbP	0.42	0.37	0.05
SeGa-PbP	0.66	0.58	0.08