Electronic, mechanical, optical and photocatalytic properties of two dimensional Janus XGaInY (X, Y = S, Se and Te) monolayers

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System	C11	C12	C66	Y	v	Status
GaS	32.11	5.99	13.06	30.98	0.20	Stable
SGaInS	23.86	5.65	9.10	22.52	0.23	Stable
SeGaInSe	20.15	4.73	7.71	19.04	0.23	Stable
TeGaInTe	17.02	3.78	6.62	16.18	0.22	Stable
SGaInSe	21.30	4.72	8.29	20.25	0.22	Stable
SeGaInS	22.88	5.69	8.59	21.47	0.25	Stable
SGaInTe	15.54	3.55	5.99	14.73	0.23	Stable
TeGaInS	21.70	5.17	8.26	20.46	0.23	Stable
SeGaInTe	17.39	3.89	6.75	16.51	0.22	Stable
TeGaInSe	18.94	4.03	7.45	18.08	0.21	Stable

Table S1 Elastic constants, Young's modulus (Y) and Poisson ratio (v) of GaS and Janus XGaInY monolayers.

Structures	Δq Ga→S	Δq In→S	Δq Ga→Se	Δq In→Se	Δq Ga→Te	Δq In→Te	Δq Ga→In
GaS	0.85 (51.56)	⋯	⋯	⋯	⋯	⋯	⋯
SGaInS	0.78 (51.55)	0.83 (51.03)	⋯	⋯	⋯	⋯	0 (0.44)
SeGaInSe	⋯	⋯	0.63 (50.32)	0.71 (49.73)	⋯	⋯	0 (0.50)
TeGaInTe	⋯	⋯		⋯	0.42 (54.70)	0.54 (54.05)	0 (0.55)
SGaInSe	0.81 (51.57)	⋯	⋯	0.66 (49.70)			0 (0.32)
SeGaInS	⋯	0.87 (51.01)	0.60 (50.27)	⋯	⋯	⋯	0 (0.63)
SGaInTe	0.82 (51.59)	⋯	⋯	⋯	⋯	0.48 (53.88)	0 (0.05)
TeGaInS	⋯	0.82 (51.00)	⋯	⋯	0.43 (54.53)	⋯	0 (0.99)
SeGaInTe	⋯	⋯	0.66 (50.43)	⋯	⋯	0.48 (53.97)	0 (0.23)
TeGaInSe	⋯	⋯	⋯	0.73 (49.79)	0.40 (54.59)	⋯	0 (0.84)

Table S2 Bader charges of all Janus monolayers. The FIC (%) values are enclosed in bracket.
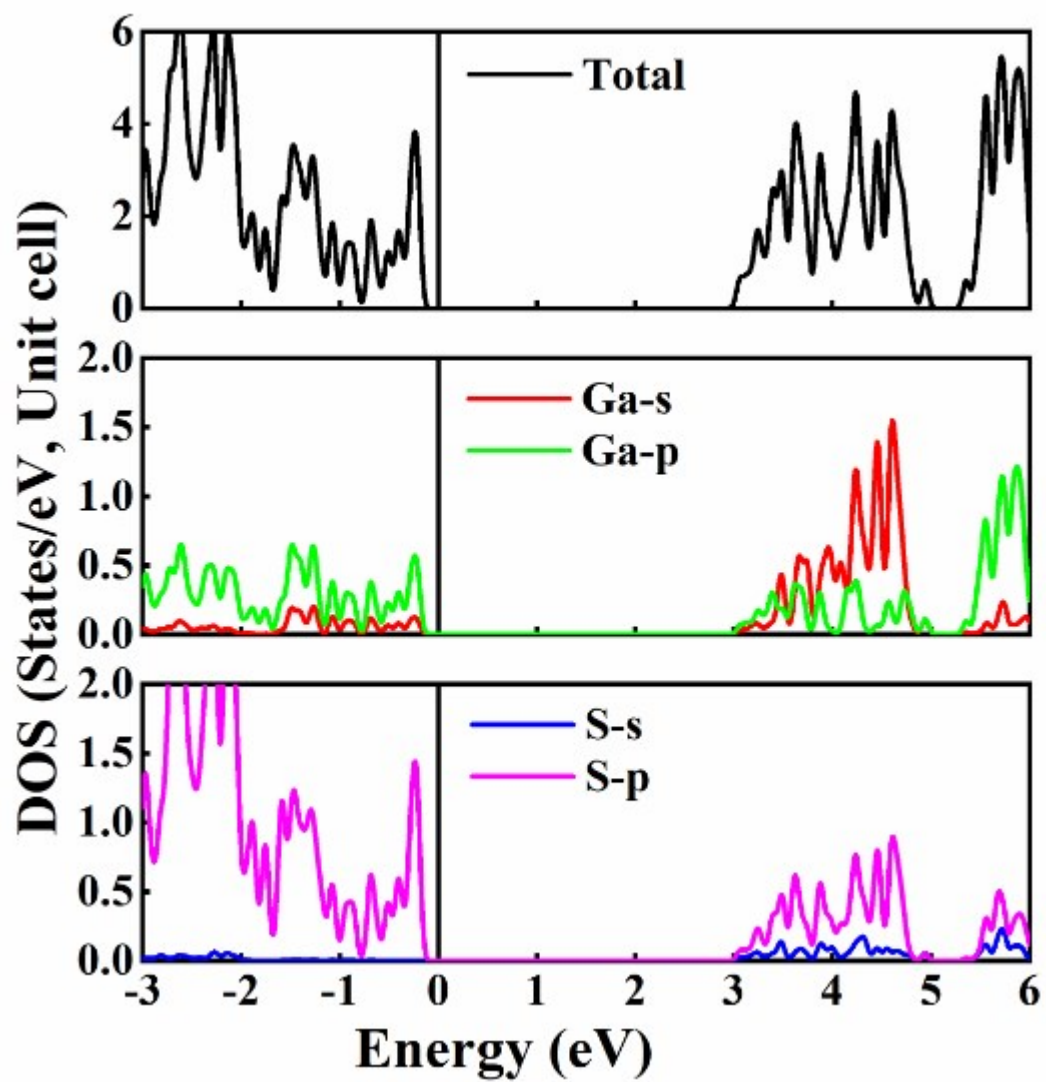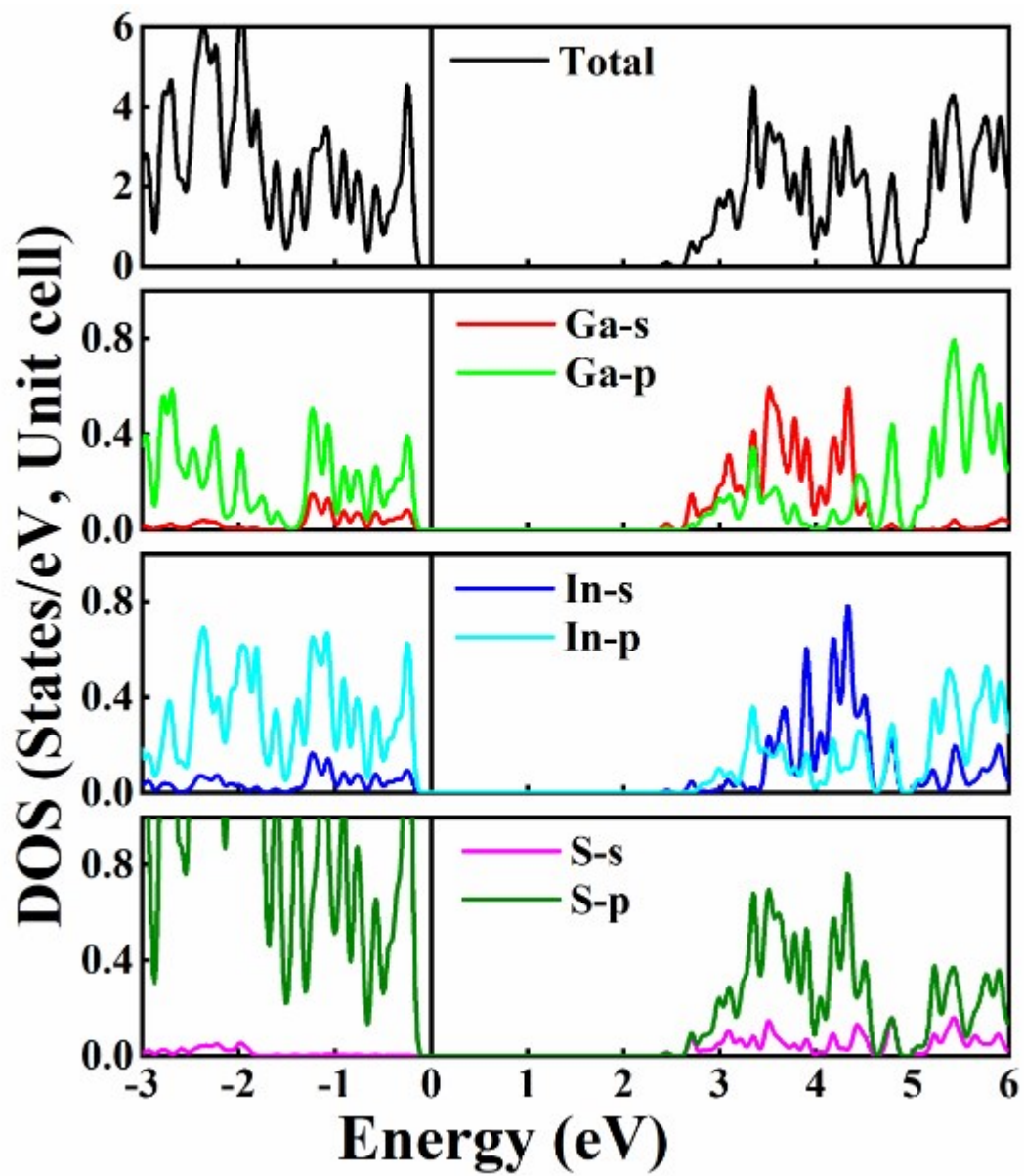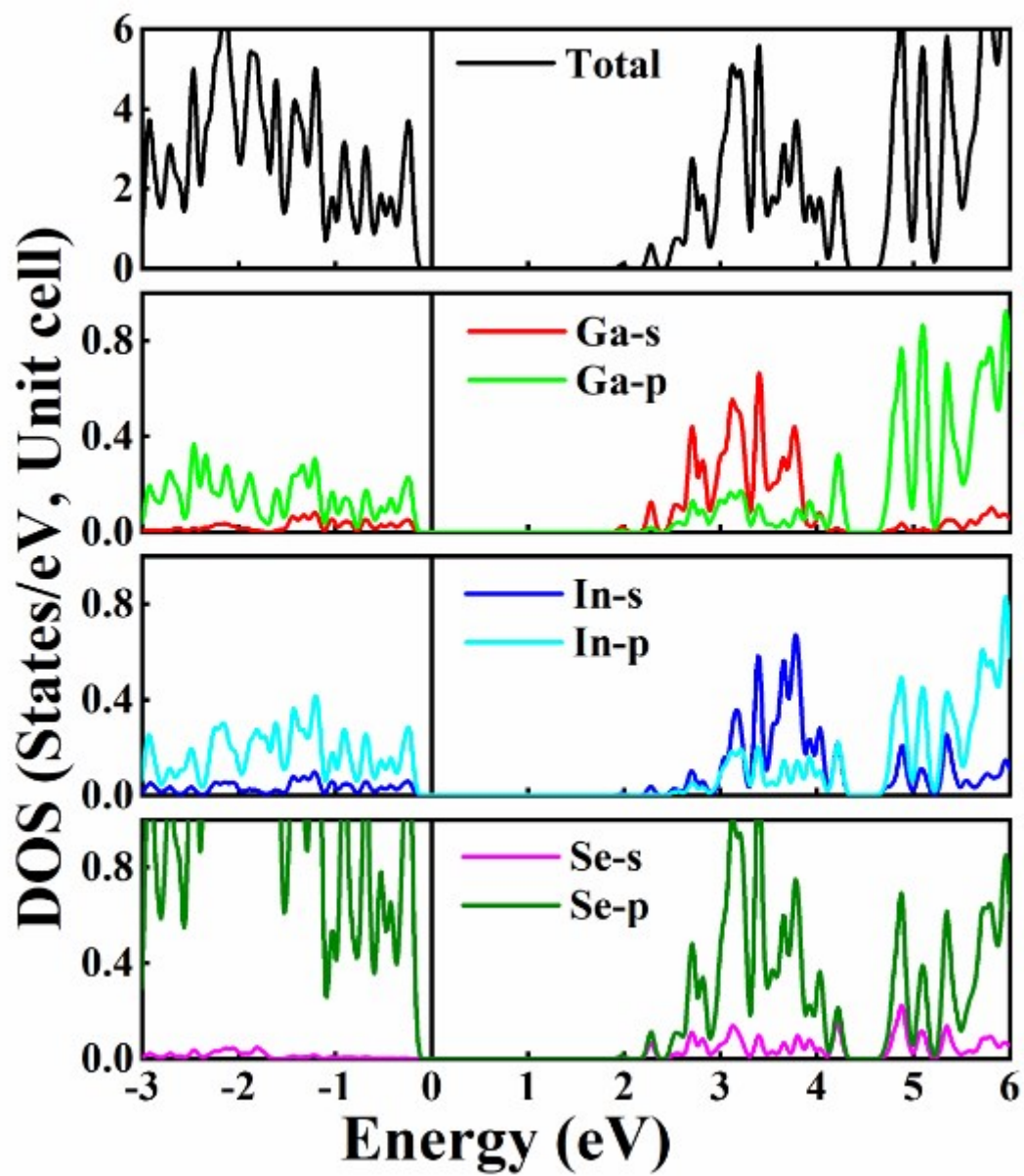
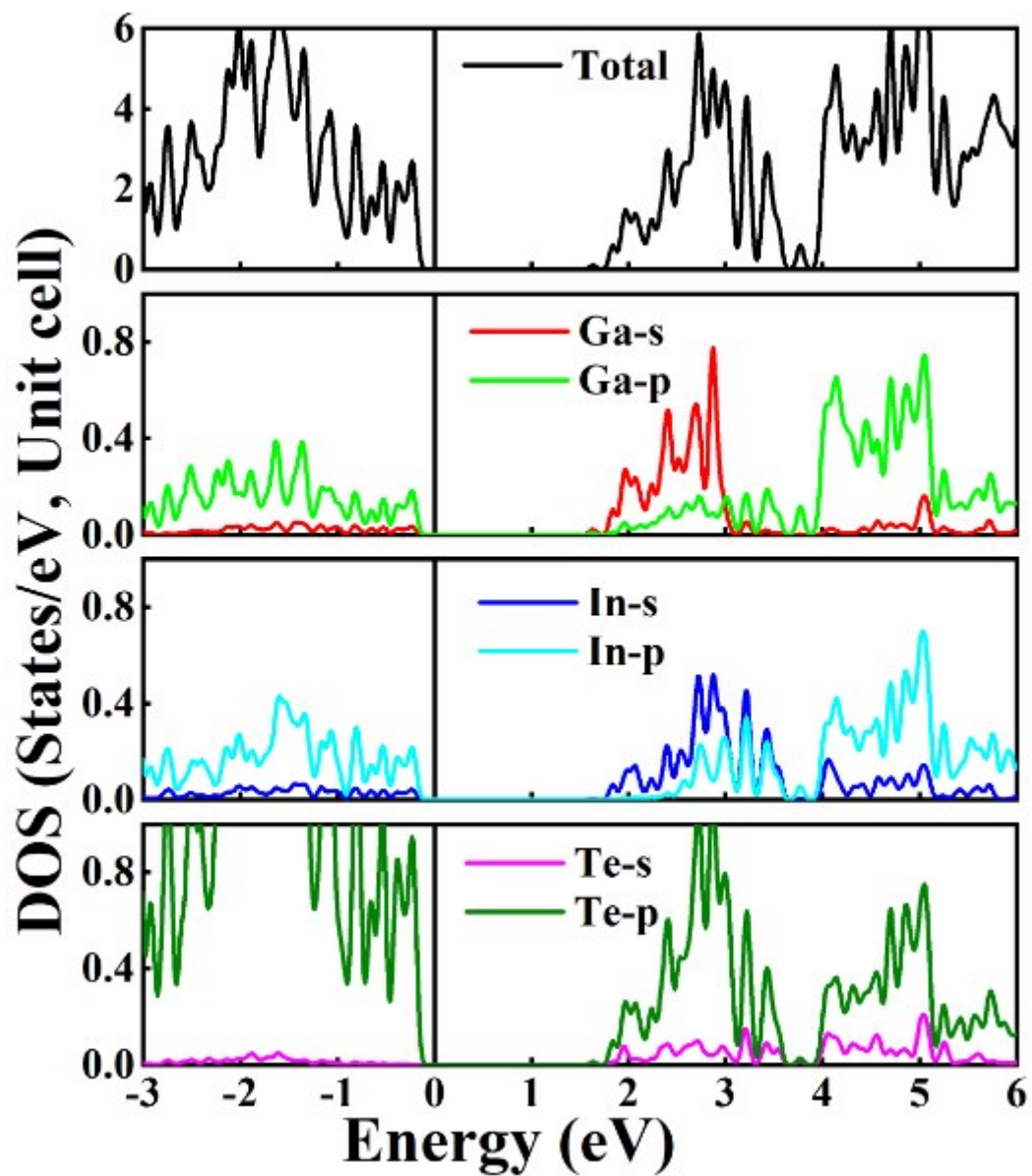Fig. S1 PDOS of GaS

Fig. S2 PDOS of SGaInS
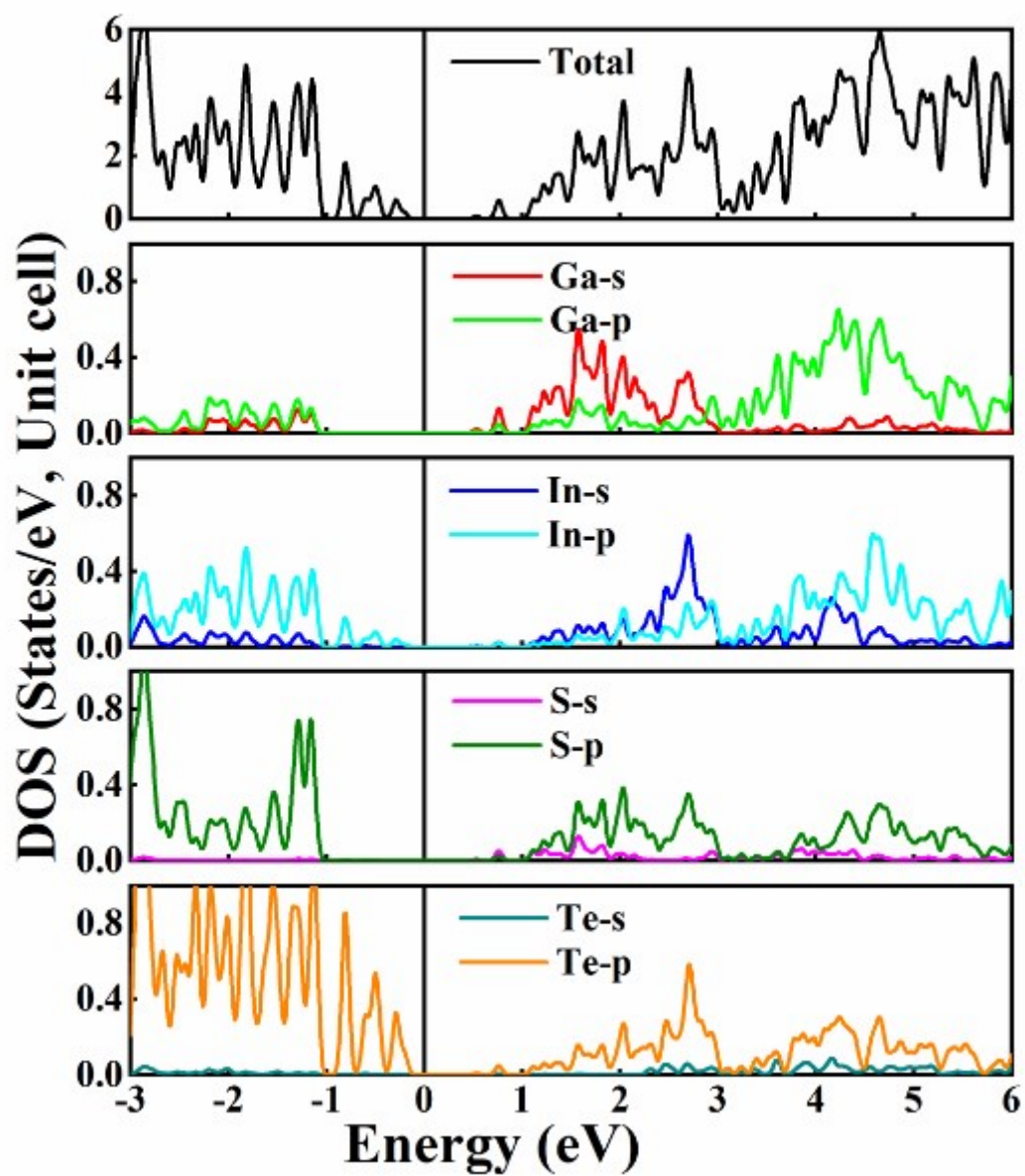
Fig. S3 PDOS of SeGaInSe

Fig. S4 PDOS of TeGaInTe
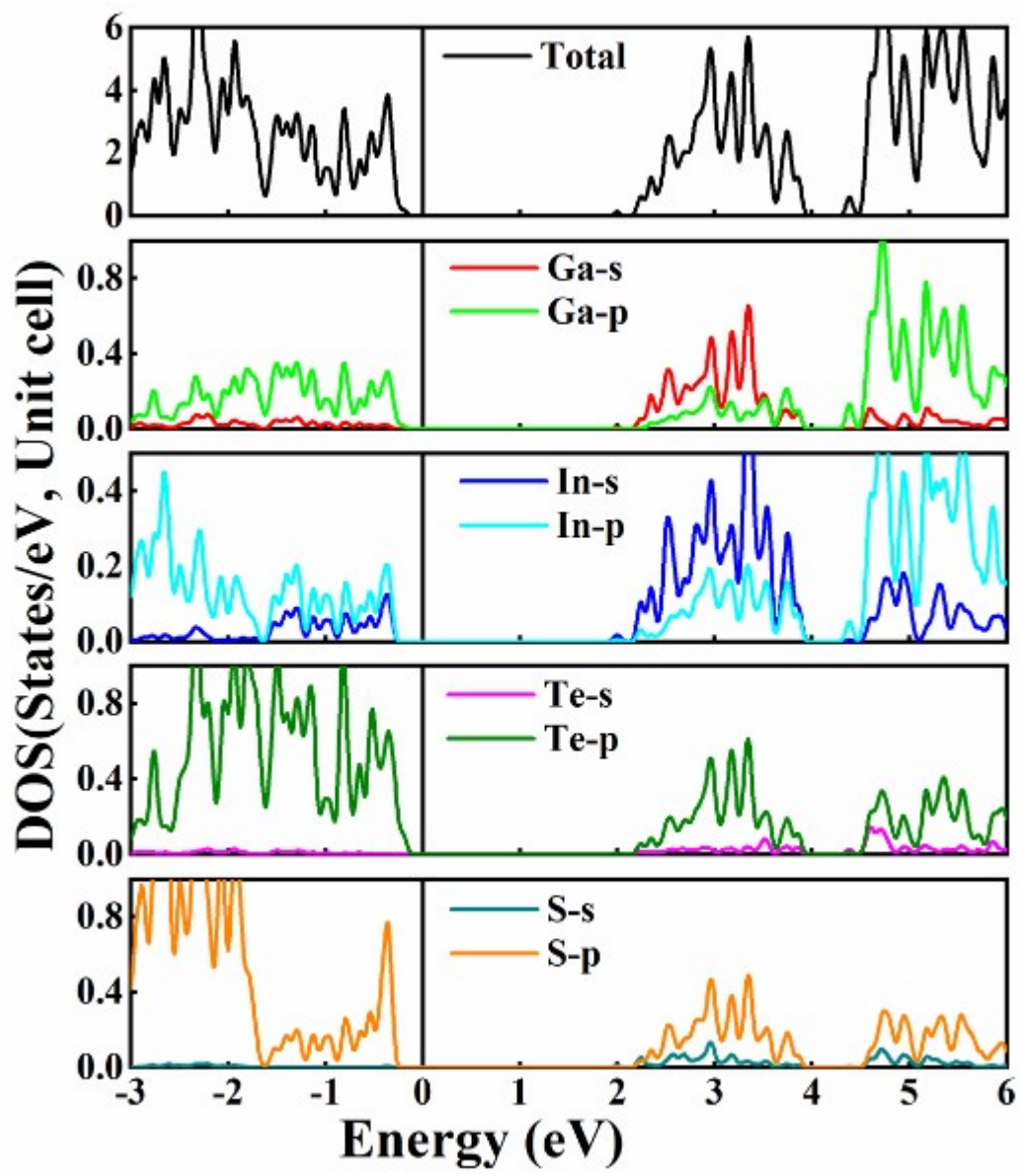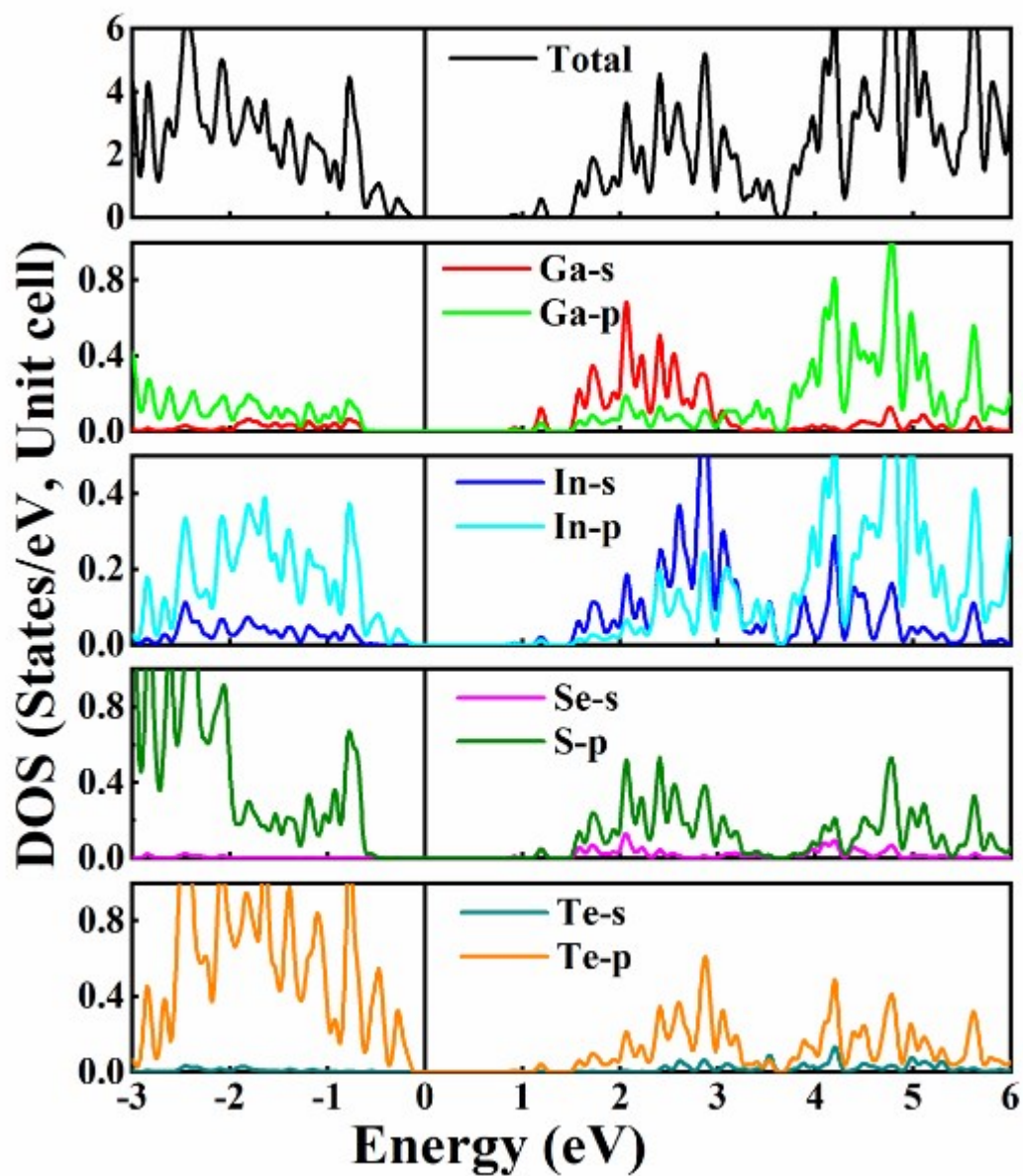
Fig. S5 PDOS of SGaInTe
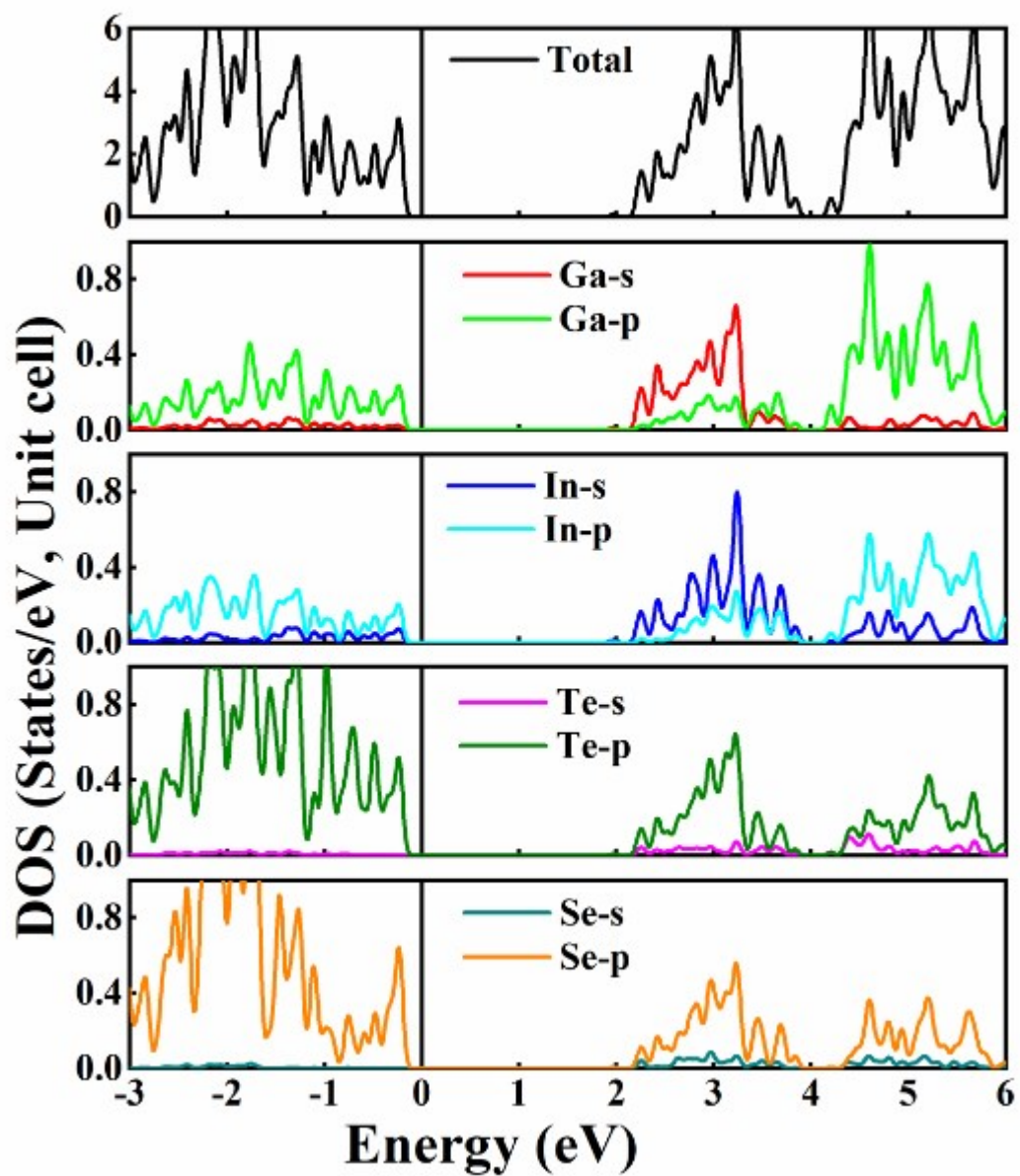
Fig. S6 PDOS of TeGaInS
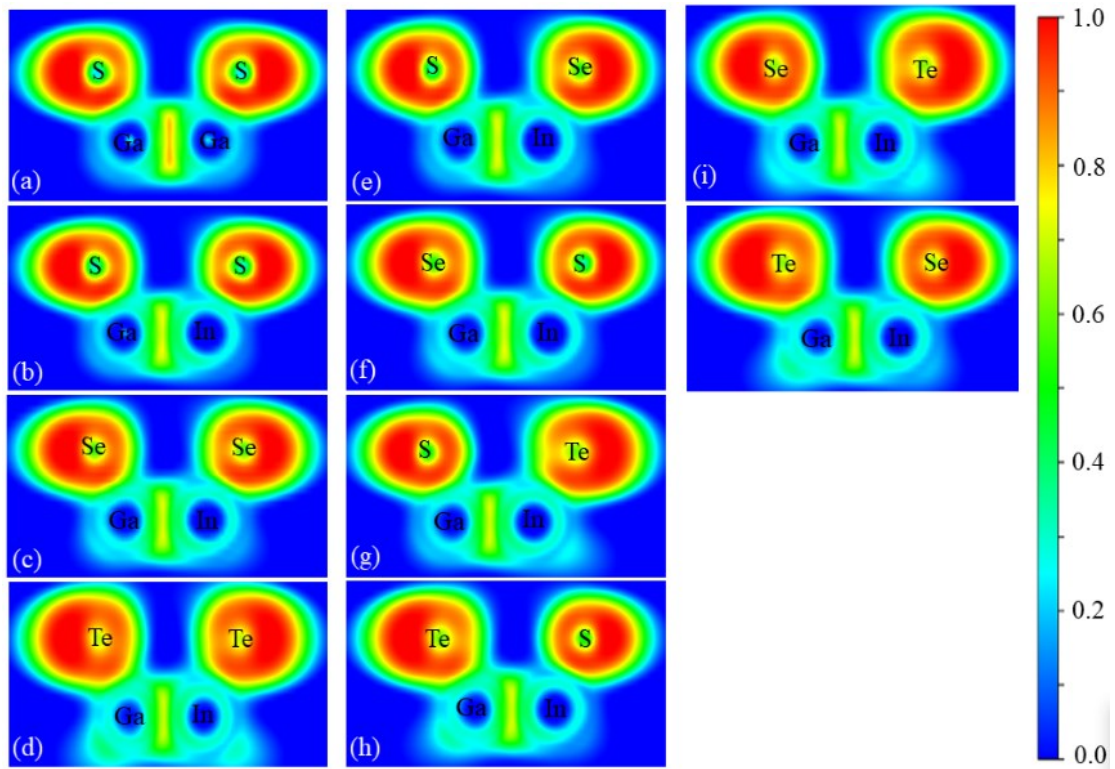
Fig. S7 PDOS of SeGaInTe

Fig. S8 PDOS of TeGaInSe

Fig. S9 ELF plot along the (110) plane of (a) single-layer GaS, and Janus (b) SGaInS, (c)SeGaInSe, (d) TeGaInTe, (e) SGaInSe, (f) SeGaInS, (g) SGaInTe, (h) TeGaInS, (i) SeGaInTe and (j) TeGaInSe monolayers.
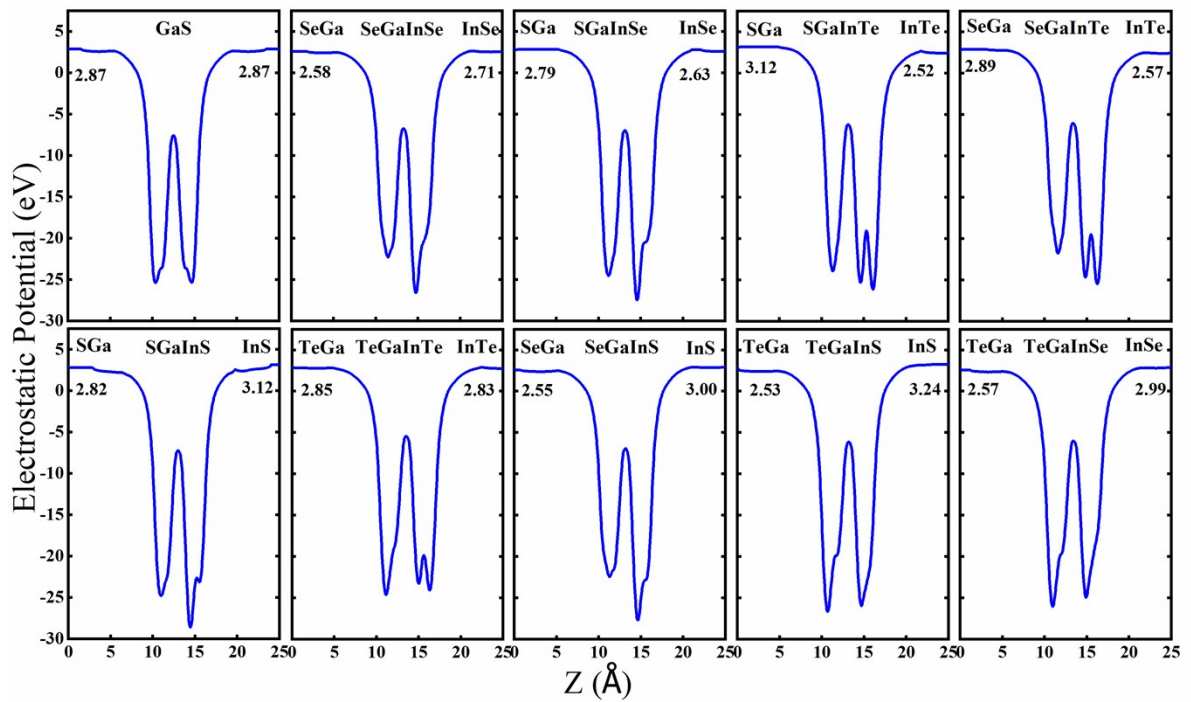

Fig. S10 The electrostatic potential of pristine and Janus XGaInY monolayers with dipole correction.