Supplementary Information

Polarity reversal and strain modulation of Janus MoSSe/GaN Polar semiconductor heterostructures

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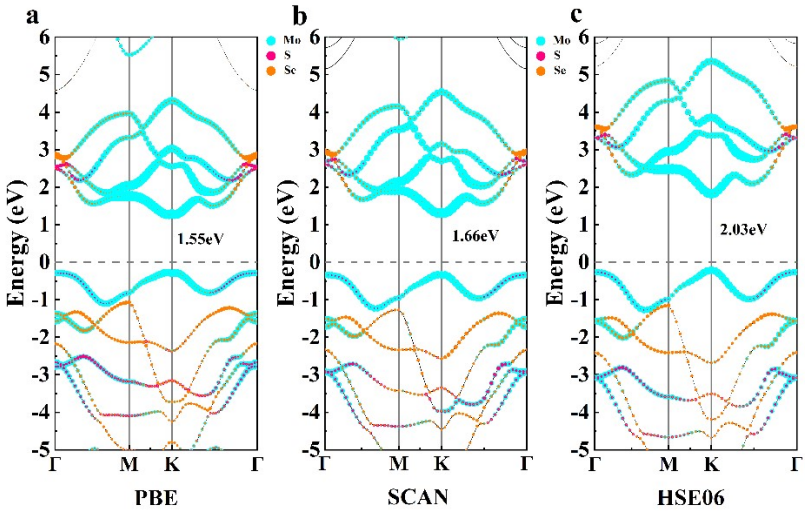

Figure S1. Calculated bandstructures of monolayer Janus MoSSe by using (a) PBE, (b) SCAN, and (c) HSE06 functionals, respectively.

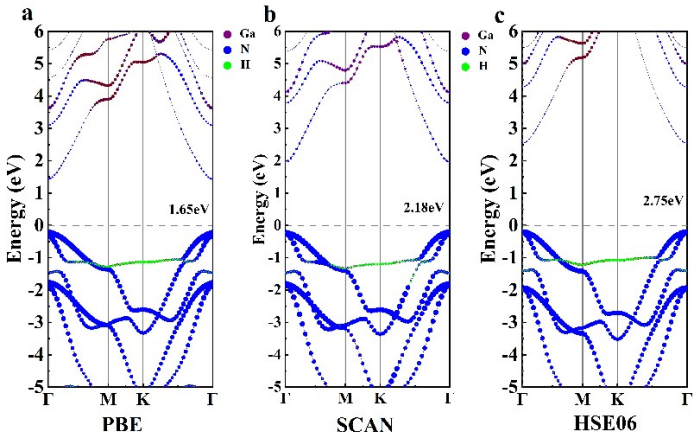

Figure S2. Calculated bandstructures of GaN by using (a) PBE, (b) SCAN, and (c) HSE06 functionals, respectively.

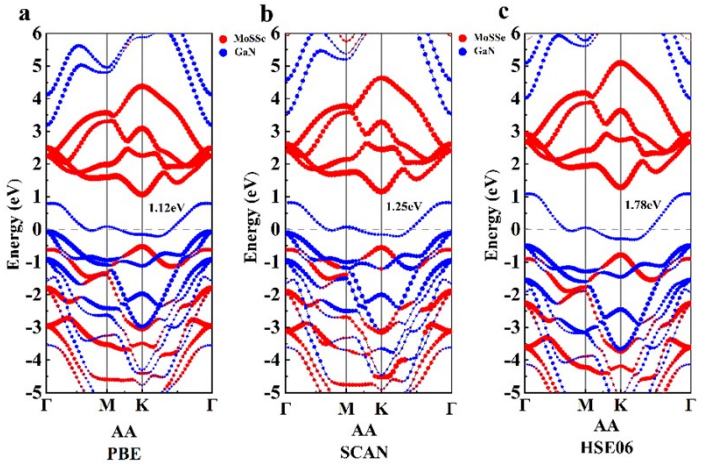

Figure S3. Calculated bandstructures of Janus MoSSe/GaN heterojunctions in AA configuration by using (a) PBE, (b) SCAN, and (c) HSE06 functionals, respectively.

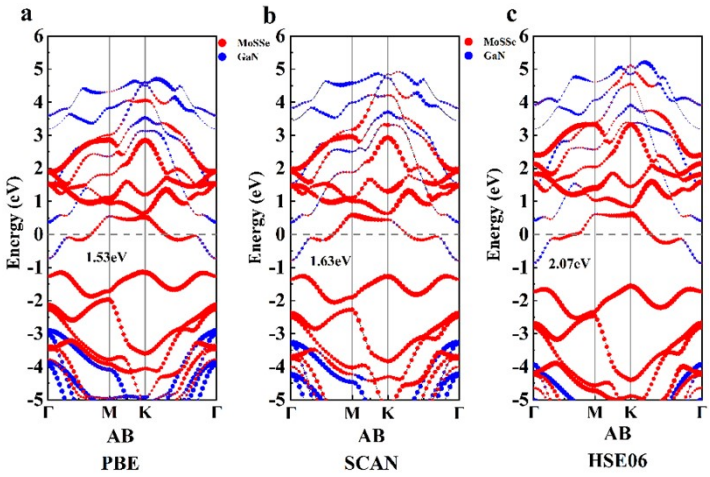

Figure S4. Calculated bandstructures of Janus MoSSe/GaN heterojunctions in AB configuration by using (a) PBE, (b) SCAN, and (c) HSE06 functionals, respectively.

Table S1. Binding energy of Janus MoSSe/GaN heterojunctions in the AA configuration and their energy before and after optimization.

AA	-10%	-6%	0	+6%	+10%
Energy before optimization (eV)	-42.89	-45.01	-	-45.32	-44.29
Energy after optimization (eV)	-43.84	-45.02	-46.01	-45.43	-44.6
Binding energy (eV)	-0.01	-0.04	-0.08	-0.35	-0.45

Table S2. Binding energy of Janus MoSSe/GaN heterojunctions in the AA' configuration and their energy before and after optimization.

AA'	-10%	-6%	0	+6%	+10%
Energy before optimization (eV)	-43.15	-45.16	-	-45.46	-44.51
Energy after optimization (eV)	-43.16	-45.17	-46.1	-45.61	-45.04
Binding energy (eV)	-0.09	-0.29	-0.17	-0.81	-1

Table S3. Binding energy of Janus MoSSe/GaN heterojunctions in the AB configuration and their energy before and after optimization.

AB	-10%	-6%	0	+6%	+10%
Energy before optimization (eV)	-44.7	-46.66	-	-46.94	-46.94
Energy after optimization (eV)	-44.7	-46.88	-47.57	-47.09	-47.09
Binding energy (eV)	-0.05	-0.15	-0.24	-0.42	-0.5

Table S4. Binding energy of Janus MoSSe/GaN heterojunctions in the AB' configuration and their energy before and after optimization.

AB'	-10%	-6%	0	+6%	+10%
Energy before optimization (eV)	-44.87	-46.84	-	-47.13	-46.22
Energy after optimization (eV)	-45.56	-47.04	-47.69	-47.33	-46.73
Binding energy (eV)	-0.2	-0.37	-0.42	-0.6	-0.69