Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Twistronics in two-dimensional TMD van der Waals interface

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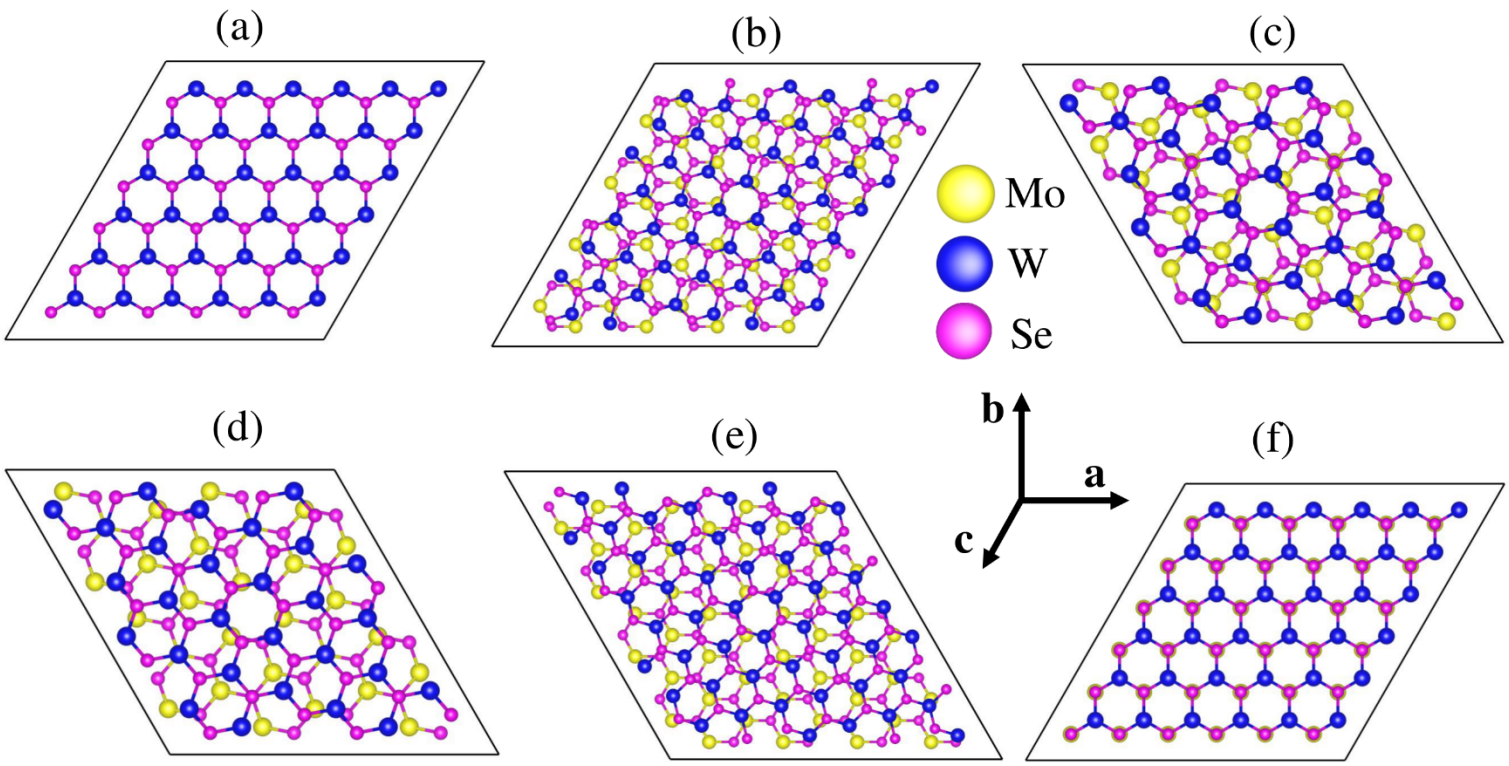

FIG. S1: The top view of twisted $MoSe_2/WSe_2$ heterostructure configuration for twist angles (a) 0°, (b) 16.10°, (c) 21.79°, (d) 43.9°, and (e) 60°

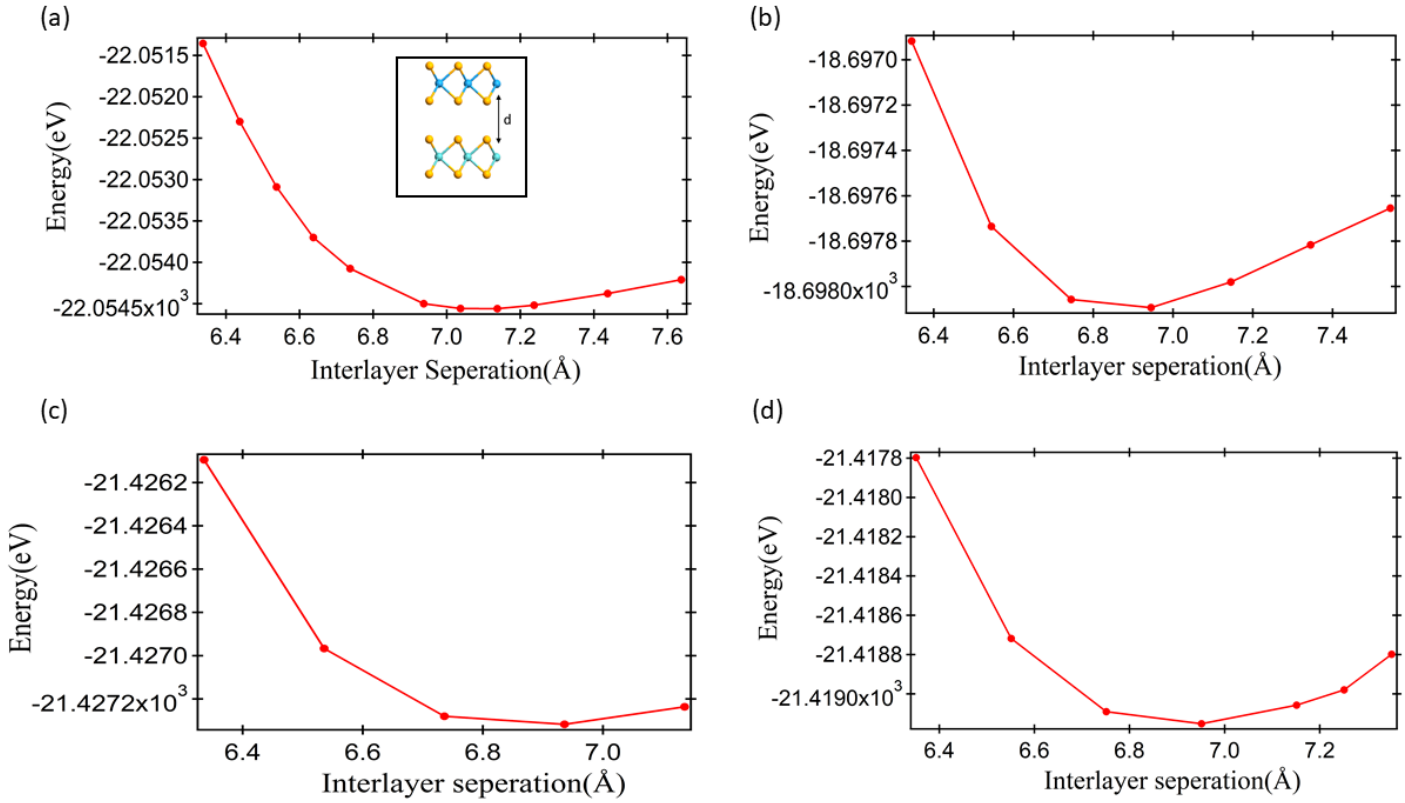

FIG. S2: Total Energy E (eV) as a function of interlayer separation d (Å) of $MoSe_2/WSe_2$, WS_2/WSe_2, $MoSe_2/WS_2$, and MoS_2/WSe_2 for $\theta = 0^o$

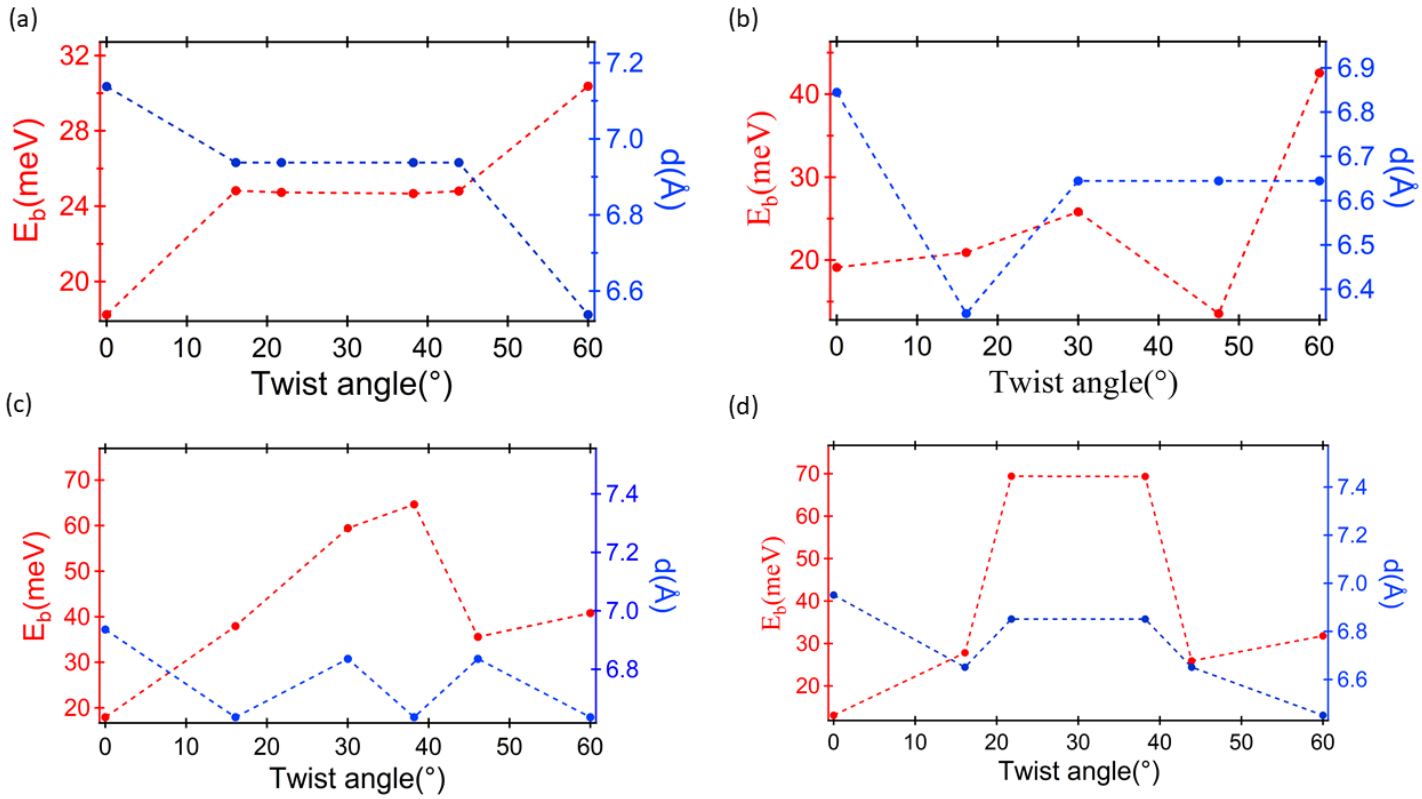

FIG.S3: Binding energy and equilibrium separation variation of $MoSe_2/WSe_2$, WS_2/WSe_2, $MoSe_2/WS_2$, and MoS_2/WSe_2 heterostructures for different twisting angles.

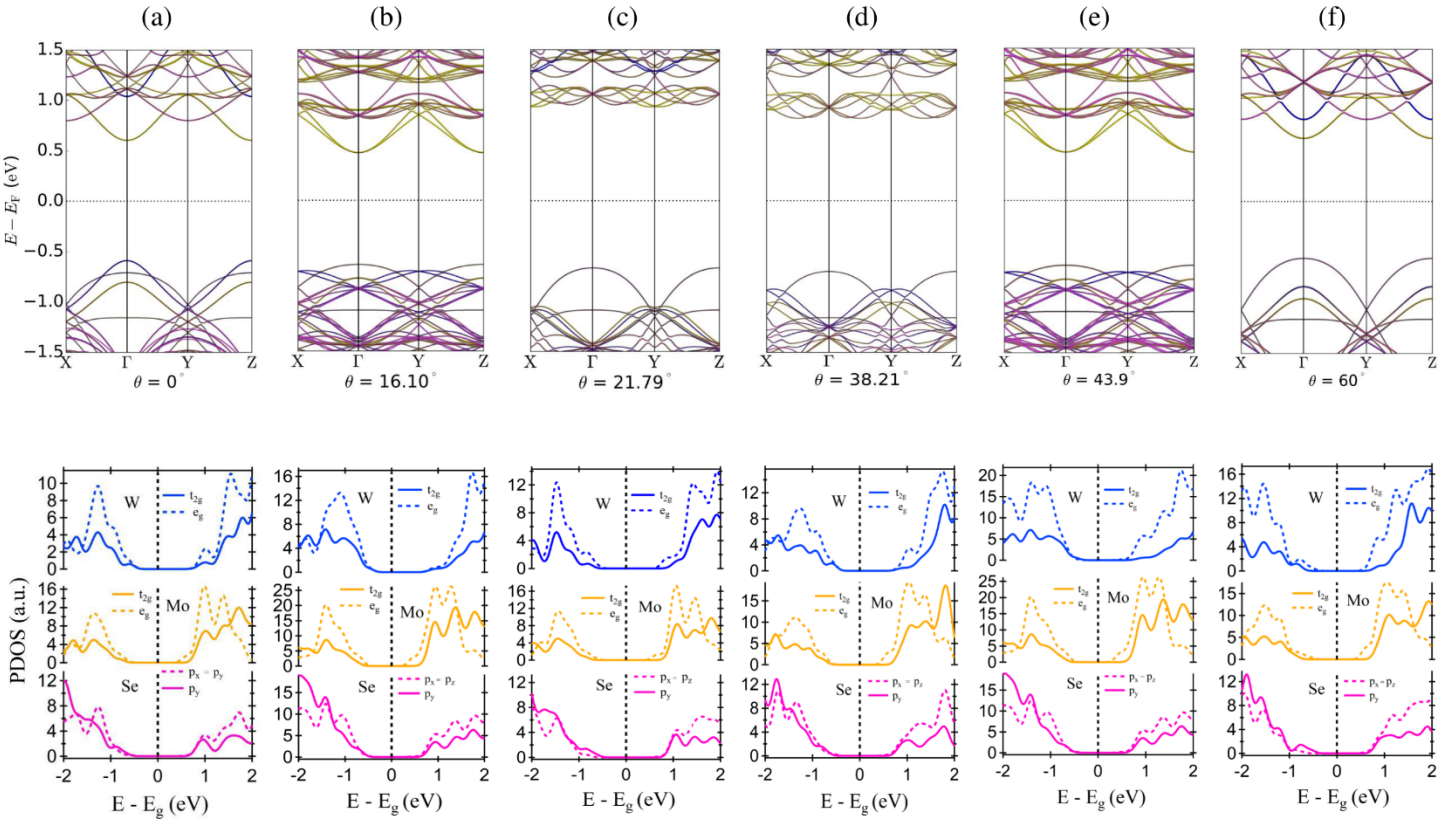

FIG. S4: The fat band structure and projected density of states of twisted $MoSe_2/WSe_2$ heterostructure for twist angles (a) 0°, (b) 16.10°, (c) 21.79°, (d) 43.9°, and (e) 60°. Yellow, blue, and pink represents band contributions from Mo, W, and Se atoms respectively.

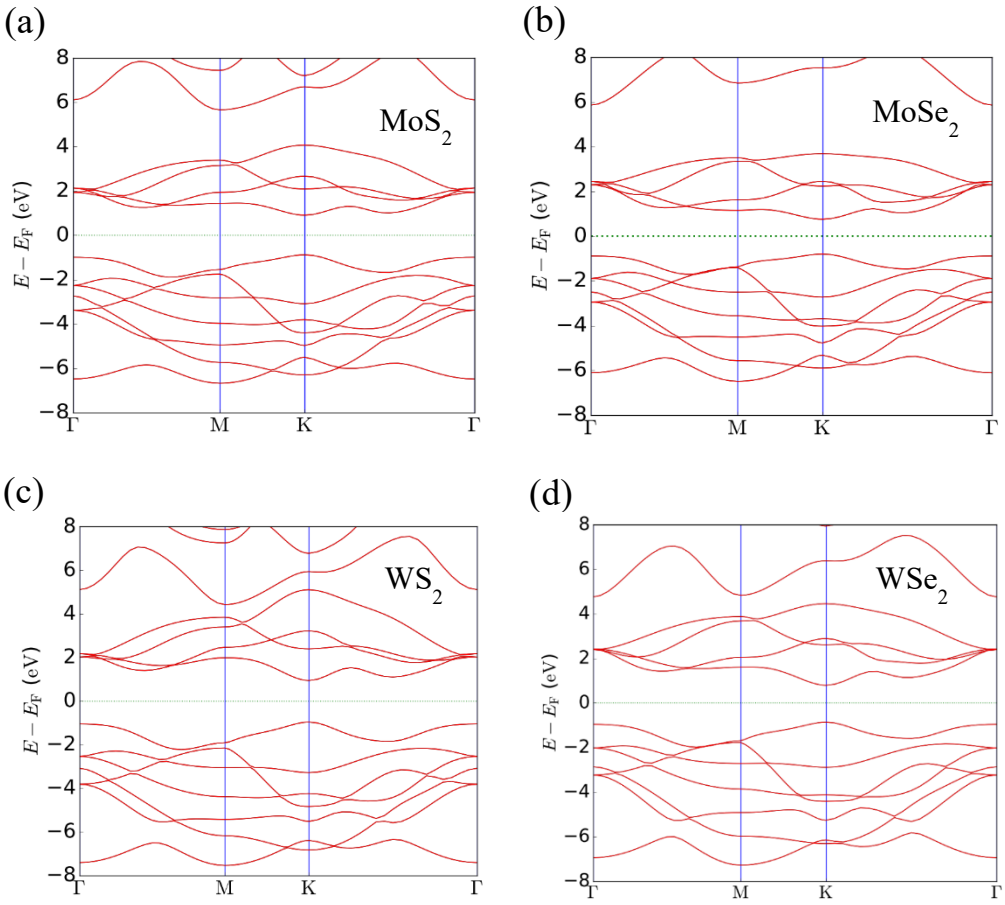

FIG. S5: The band structure of (a) MoS_2, (b) $MoSe_2$, (c) WS_2, and (d) WSe_2, calculated by PBE method.

Table S1: The comparison of band gap values calculating using PBE method with experimental result:

Material	Method	E_g (eV)
MoS_2	PBE	1.78
	Expt.	1.90
$MoSe_2$	PBE	1.56
	Expt.	1.57
WS_2	PBE	1.90
	Expt.	1.94-1.99
WSe_2	PBE	1.64
	Expt.	1.65

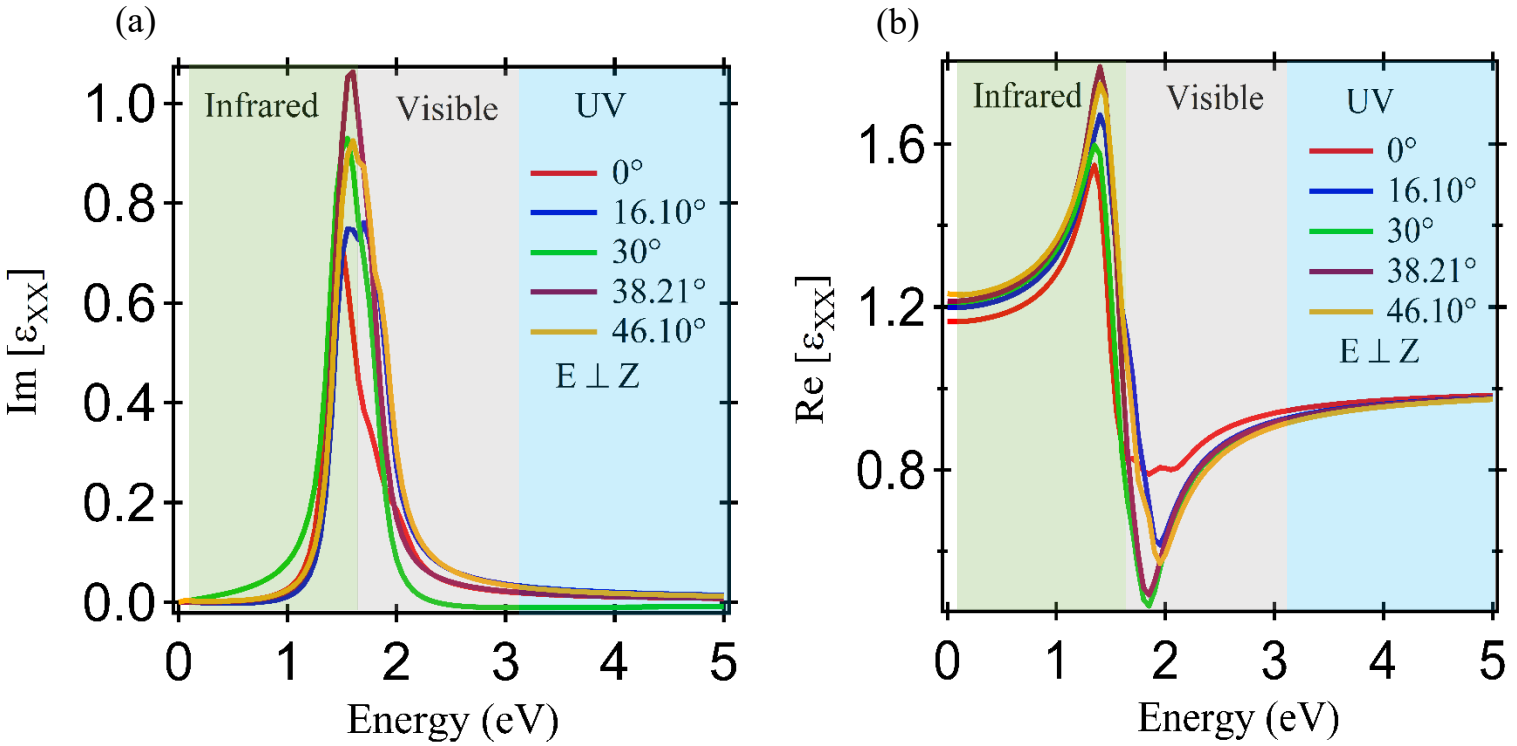

FIG. S6: (a)Variation of imaginary part of dielectric constant $\varepsilon_1(\omega)$, and (b) real part of dielectric constant $\varepsilon_2(\omega)$ plotted as a function of photon energy (0-5 eV) along x-direction for $MoSe_2/WS_2$ heterostructure with different twist angle.

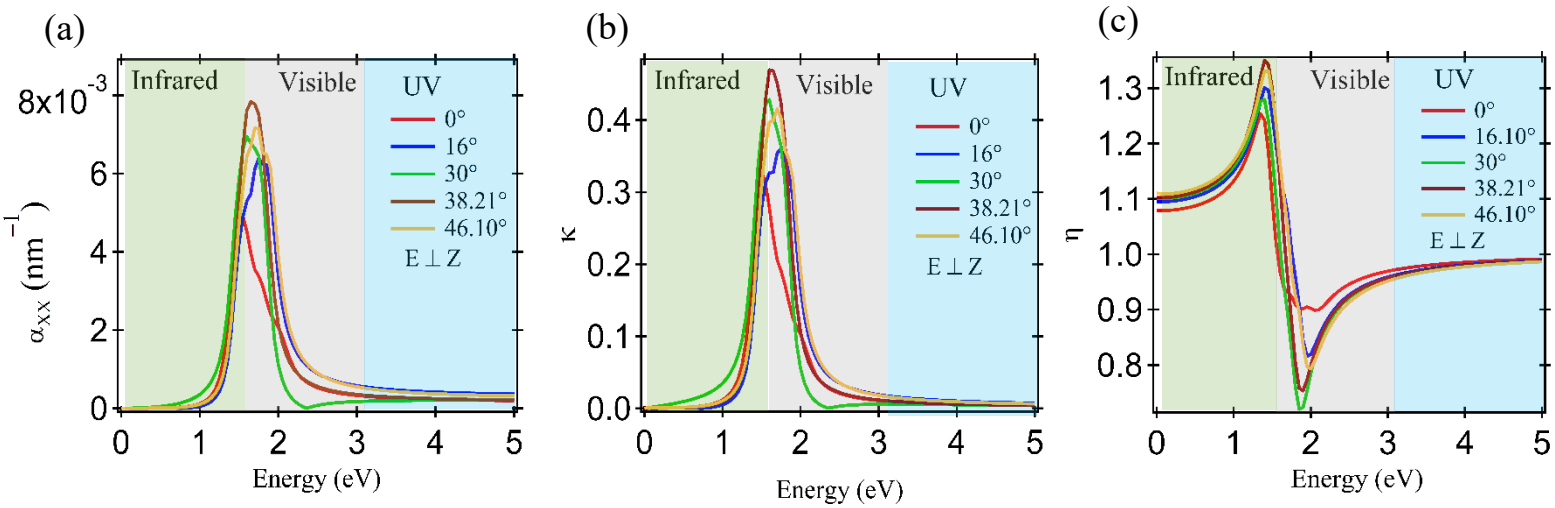

Figure S7: (a) Refractive index (η), (b) Extinction coefficient (κ), and (c) Absorption coefficient (α), plotted as a function of photon energy (0-5 eV) along x-direction for $MoSe_2/WS_2$, heterostructure with different twist.