Supplementary Information (SI) for Dalton Transactions.
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Supporting Information

Tunable Transport Mode of Polaron in Polarized Janus MoSSe Few-Layers: A Constrained Density Functional Theory Study

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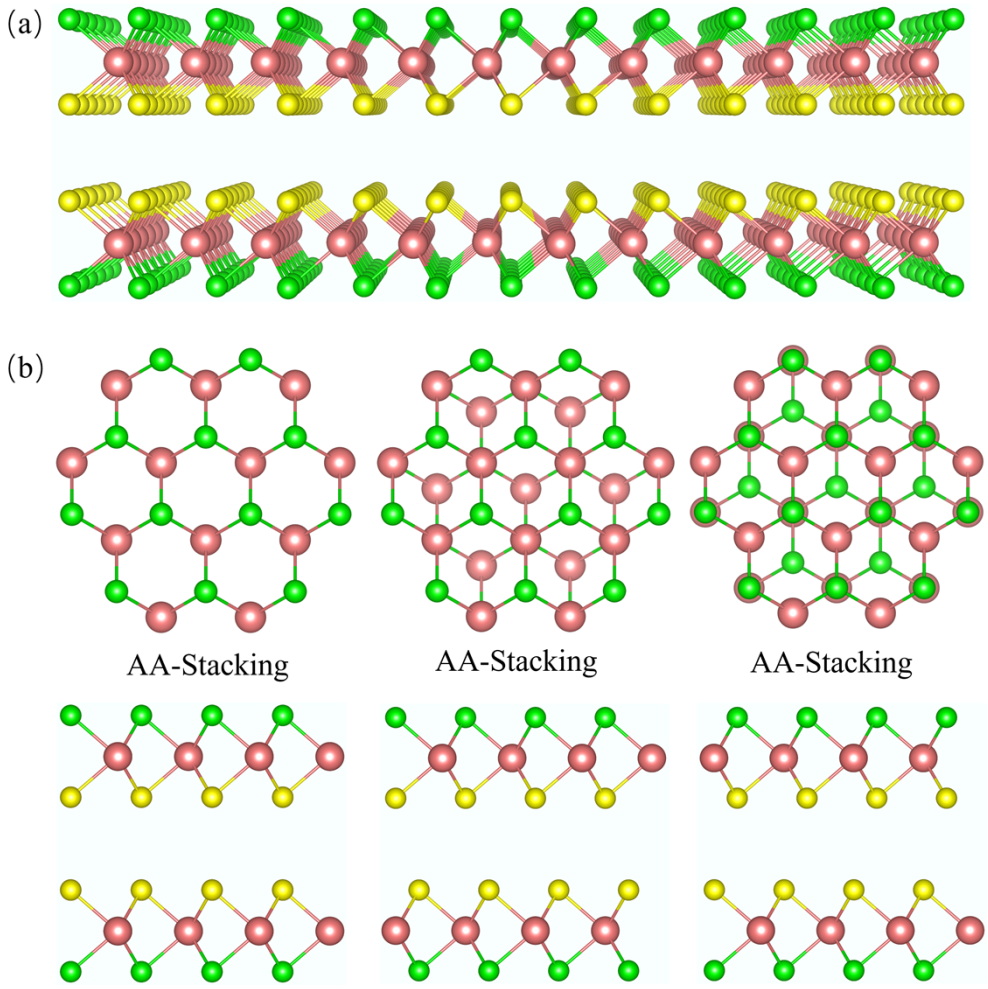
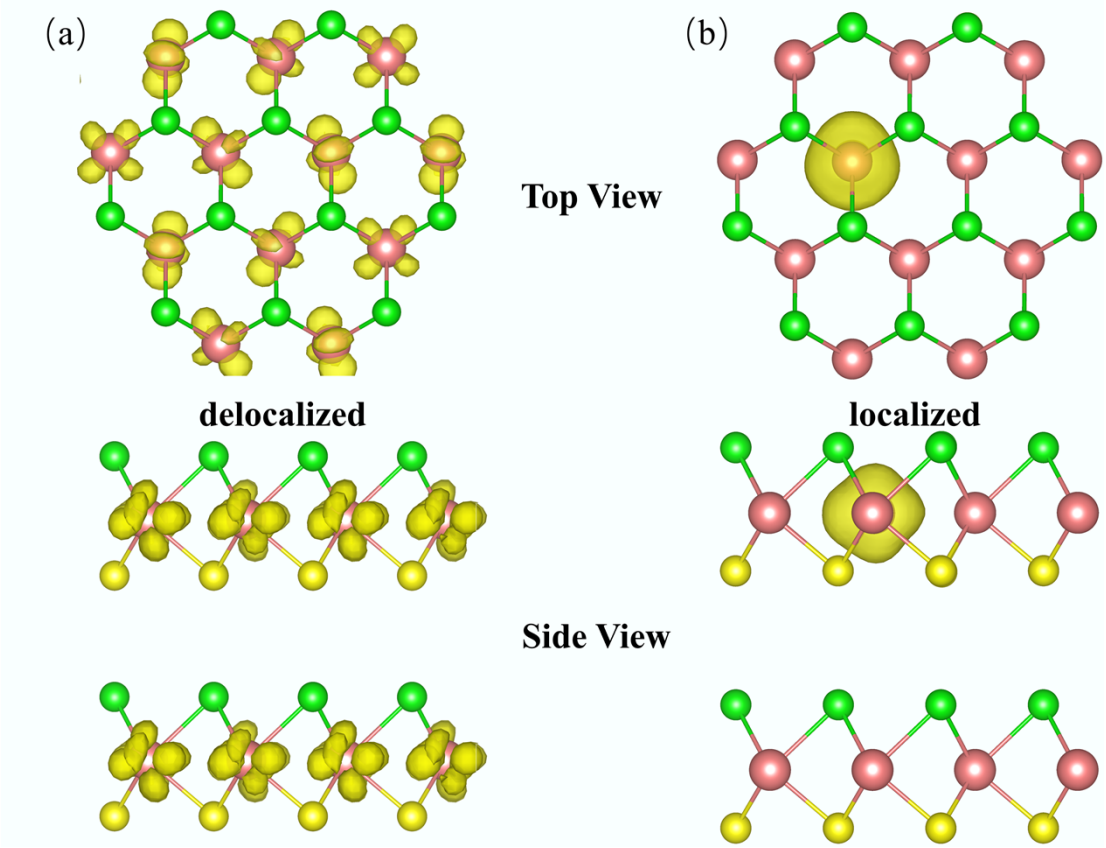
S1: SeMoS/SMoSe combination



SI-Fig. 1*. (Color online) (a) The structure of the SeMoS/SMoSe heterostructure. (b) The top and side views of the AA-, AB-, and AC-stackings of the SeMoS/SMoSe heterostructure.*

S2: Delocalized and localized states of electron in two-layer heterostructures



SI-Fig. 2. *(Color online) (a) Delocalized states of electron in two-layer heterostructures. (b) Localized states of the small electron polaron in two-layer heterostructures.*

Table S1. *The formation energy of electrons and hole polarons varies with the size of the supercell of MoSSe monolayer .*

System	***E_{pol} (e) (eV)***	***E_{pol} (h) (S)(eV)***	***E_{pol} (h) (Se)(eV)***
MoSSe(3*3)	0.30	1.45	1.33
MoSSe(4*4)	0.34	1.38	1.27
MoSSe(5*5)	0.35	1.41	1.33
MoSSe(6*6)	0.38	1.49	1.38

Table S2. *The polaron formation energy of the MoS_2 and MoSSe monolayers.*

System	***Polaron***	***E_{pol} (eV)***	***E_{el} (eV)***	***E_{st} (eV)***
MoS_2	*Electron*	0.33	0.35	0.02
	Hole	1.37	1.43	0.06
MoSSe	*Electron*	0.35	0.38	0.03
	Hole (S)	1.41	1.46	0.05
	Hole (Se)	1.33	1.48	0.15