

Title: The Tunable Dipole and Carrier Mobility for Few Layer Janus MoSSe

Structure

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Supporting Information

Table. S1. The carrier mobility of few layer MoSSe predicted by theoretical calculations at 300 K. The m_e^* (m_h^*), E_e (E_h), and μ_e (μ_h) indicate the effective mass, deformation potential, carrier mobility for the electron at CBM (hole at VBM), C_{2D} is the elastic moduli along the x direction. It should be mentioned that we use AC-stacking mode to model the structure as the thickness larger than one layer. The few layer MoS₂ structures are also presented for comparison.

System	Thickness (layers)	m_e^* (m_0)	m_h^*	E_e (eV)	E_h	C_{2D} (Jm ⁻²)	μ_e (cm ² V ⁻¹ s ⁻¹)	μ_h
MoS ₂	1	0.53	0.59	7.26	1.36	136.01	160.6	2047.8
	2	0.65	0.61	3.71	3.84	363.30	1897	1111
	3	0.62	0.60	2.58	2.34	542.2	5999	5218
MoSSe	1	0.60	0.73	10.27	4.68	145.6	73.8	157.2
	2	0.57	0.7	3.46	1.73	239	1194	2915.6
	3	0.57	0.9	10.30	1.35	364	205	5894
	4	0.49	0.87	3.15	2.71	486.6	2443.2	2052