Supporting Information for: High-throughput Screening and Classification of Layered Di-Metal Chalcogenides

Table S1. The setup for generating the Monkhorst-Pack k-point meshes of 24 listed LDCs in Table 2.

Compounds		Number of k points			Compounds		Number of k points		
		b_1	b_2	b_3			b_1	b_2	b_3
1	$CsAg_3Se_2$	8	8	4	13	Cu_3TlSe_2	8	4	4
2	KAgSe	8	8	4	14	$Cs_3Bi_7Se_{12}$	4	4	4
3	KCuSe	8	8	4	15	$BaCu_2S_2$	8	8	6
4	$Rb_2Ag_4S_3$	8	8	8	16	$BaCu_2Se_2$	8	8	6
5	$CsAg_3S_2$	8	4	4	17	$MgAl_2S_4$	6	6	6
6	KCu_3S_2	8	4	4	18	$ZnIn_2S_4$	7	3	3
7	$RbCu_3S_2$	8	8	8	19	$Ba_3Zr_2S_7$	8	8	4
8	KAg_3Se_2	8	4	4	20	Ba_2ZrS_4	8	8	4
9	$RbAg_3Se_2$	8	4	4	21	$Ba_4Zr_3S_{10}$	6	6	6
10	$K_2Ag_4Se_3$	8	8	8	22	$TlInS_2$	10	10	2
11	RbNaS	8	8	6	23	Bi_2PbSe_4	5	5	5
12	Cu_3TlS_2	8	8	8	24	$Bi_2Pb_2Se_5$	8	8	2

Table S2. The in-plane direction which has the smallest effective mass and the corresponding effective mass of the LDCs in Fig. 6. As a result of the small effective mass, the carrier mobility along that in-plane direction may be high.

Compounds	Carrier Type	k path	Effective mass (m_0)
$BaCu_2S_2$	electron	Γ-X	0.20
Ba_2ZrS_4	electron	Γ-X	0.20
KAgSe	electron	Γ-X	0.17
Cs_3Bi_7Se	electron	Y-X_1	0.22
	hole	Y-X_1	0.26
$Rb_2Ag_4S_3$	electron	Γ-N	0.15
	hole	Γ-X	0.16
$TlInS_2$	electron	K-M	0.31
	hole	Γ-A	0.16
Bi_2PbSe_4-bulk	electron	Z-P_1	0.12
	hole	Z-P_1	0.24
$MgAl_2S_4$-bulk	electron	Γ-X	0.24
	hole	Γ-L	0.36
$ZnIn_2S_4$-bulk	electron	Γ-Y	0.21
	hole	Γ-Y	0.21
Bi_2PbSe_4-monolayer	electron	Γ-M	0.22
	hole	Γ-M	0.62
$MgAl_2S_4$- monolayer	electron	Γ-K	0.24
	hole	Γ-K	0.40
$ZnIn_2S_4$- monolayer	electron	Γ-K	0.24
	hole	Γ-K	0.34