Supplementary Material

Breaking the Boltzmann Limit in Sub-5 nm Monolayer CdPS₃ Transistors

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1. *I*-V_g curves along the (a) armchair and (b) zigzag directions at different doping concentrations.

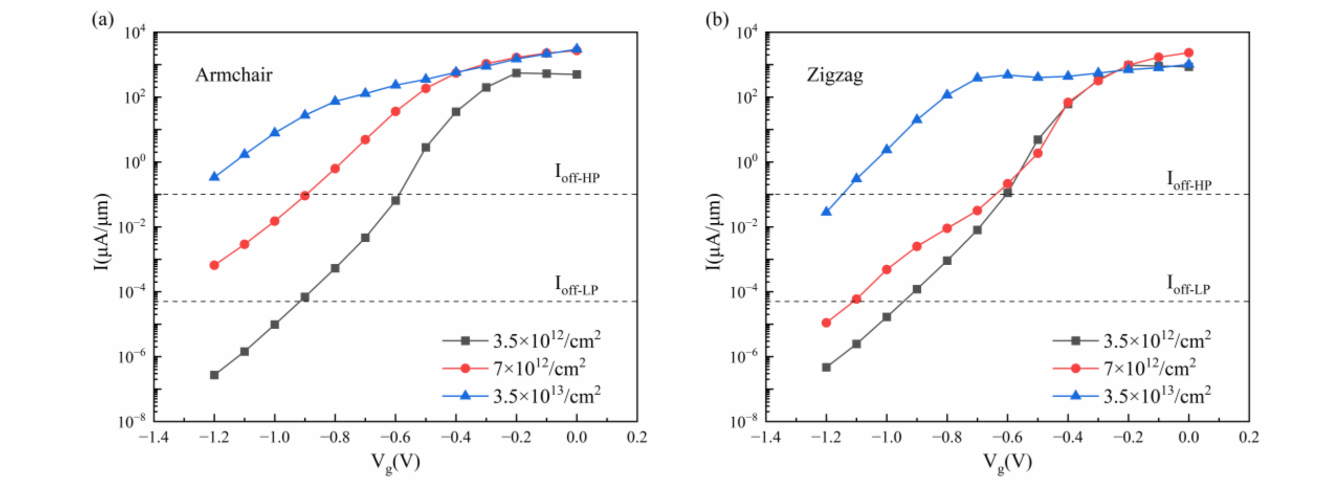

FIG. S1. *I*-V_g curves along the (a) armchair and (b) zigzag directions at different doping concentrations.

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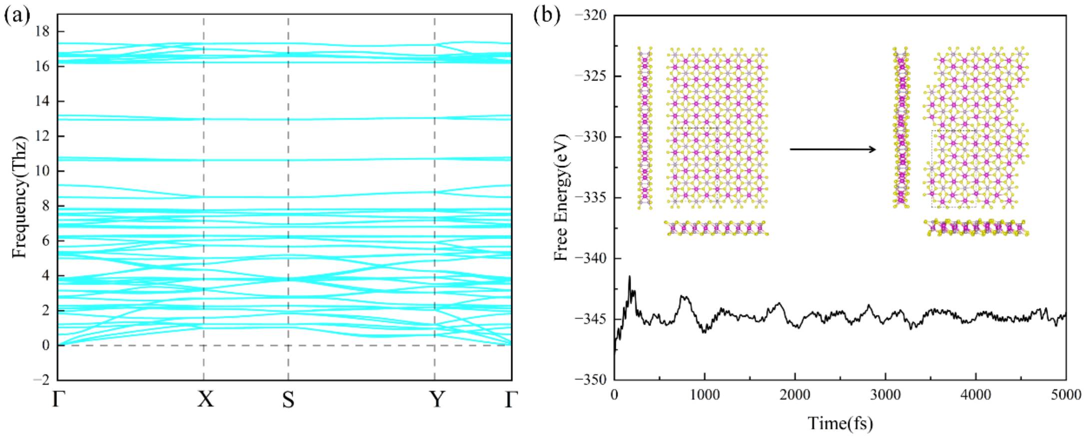

Fig. S2. (a) The phonon dispersion spectra of $CdPS_3$. (b) The free energy as a function of time during ab initio molecular dynamics (AIMD) simulation of $CdPS_3$ at 300 K. The inset shows the atomic structure of $CdPS_3$ before and after heating at 300 K for 5,000 fs.

TABLE S I. Performance details of monolayer $CdPS_3$ transport devices along the armchair direction under ITRS HP standards (off-state current $I_{off} = 0.1\ \mu A/\mu m$). Dielectric constant (K), gate length (L_g), underlap (UL), on-state current (I_{on}), subthreshold swing (SS), intrinsic delay time (τ), power-delay product (PDP).

k	L_g(nm)	UL(nm)	$I_{on}(\mu A/\mu m)$	SS(mV/dec)	$\tau(ps)$	$PDP(fJ/\mu m)$
3.9	5	0	1250	113	0.212	0.17
		1	2020	83	0.108	0.139
		2	1380	78	0.168	0.148
	3	1	744	147	0.244	0.116
		2	991	116	0.165	0.104
		3	657	103	0.263	0.11
	2	2	707	157	0.201	0.09
		3	560	116	0.246	0.088
	1	3	459	153	0.241	0.071
		4	311	131	0.354	0.071
25	5	0	2680	98	0.131	0.225
		1	2800	79	0.12	0.216
		2	2180	74	0.15	0.21
	3	1	1400	126	0.183	0.164
		2	1730	101	0.155	0.171
		3	1320	92	0.189	0.16
	2	2	1190	133	0.165	0.125
		3	560	116	0.257	0.092
	1	3	867	130	0.2	0.111
		4	779	111	0.238	0.118
ITRS HP	5.1	-	900	-	0.423	0.24

TABLE S II. Performance details of monolayer $CdPS_3$ transport devices along the zigzag direction under ITRS HP standards (off-state current $I_{off} = 0.1\ \mu A/\mu m$). Dielectric constant (K), gate length (L_g), underlap (UL), on-state current (I_{on}), subthreshold swing (SS), intrinsic delay time (τ), power-delay product (PDP).

k	L_g(nm)	UL(nm)	$I_{on}(\mu A/\mu m)$	SS(mV/dec)	$\tau(ps)$	$PDP(fJ/\mu m)$
3.9	5	0	2450	79	0.132	0.207
		1	2130	72	0.137	0.187
		2	1270	55	0.217	0.177
	3	1	1120	103	0.186	0.134
		2	794	52	0.217	0.11
		3	323	71	0.512	0.106
	2	2	750	245	0.211	0.101
		3	243	64	0.585	0.091
	1	3	172	94	0.606	0.067
		4	54	169	2.103	0.073
25	5	0	2380	62	0.16	0.243
		1	2520	51	0.137	0.222
		2	1900	38	0.213	0.259
	3	1	1480	95	0.17	0.161
		2	1590	57	0.169	0.172
		3	1170	48	0.219	0.164
	2	2	1340	139	0.19	0.163
		3	361	64	0.768	0.178
	1	3	812	87	0.233	0.121
		4	64	107	1.593	0.065
ITRS HP	5.1	-	900	-	0.423	0.24

Table S III. Performance details of monolayer $CdPS_3$ transport devices along the armchair direction under IRDS HP standards (off-state current $I_{off} = 0.01\ \mu A/\mu m$). Dielectric constant (K), gate length (L_g), underlap (UL), on-state current (I_{on}), subthreshold swing (SS), intrinsic delay time (τ), power-delay product (PDP).

k	L_g(nm)	UL(nm)	$I_{on}(\mu A/\mu m)$	SS(mV/dec)	$\tau(ps)$	$PDP(fJ/\mu m)$
3.9	5	0	693	112	0.377	0.167
		1	1318	84	0.199	0.168
		2	1093	79	0.218	0.152
	3	1	275	145	0.647	0.114
		2	645	116	0.265	0.109
		3	463	103	0.354	0.105
	2	2	135	179	0.935	0.081
		3	354	133	0.365	0.083
	1	3	-	152	-	-
		4	-	131	-	-
25	5	0	1243	105	0.274	0.218
		1	2121	76	0.162	0.22
		2	1878	74	0.182	0.218
	3	1	356	137	0.66	0.15
		2	1121	102	0.221	0.159
		3	1046	87	0.246	0.165
	2	2	334	131	0.545	0.116
		3	895	109	0.25	0.143
	1	3	322	130	0.525	0.108
		4	467	111	0.396	0.118
IRDS HP	12	-	924	75	0.78	0.47

Table S IV. Performance details of monolayer $CdPS_3$ transport devices along the zigzag direction under IRDS HP standards (off-state current $I_{off} = 0.01\ \mu A/\mu m$). Dielectric constant (K), gate length (L_g), underlap (UL), on-state current (I_{on}), subthreshold swing (SS), intrinsic delay time (τ), power-delay product (PDP).

k	L_g(nm)	UL(nm)	I_{on}($\mu A/\mu m$)	SS(mV/dec)	$\tau(ps)$	PDP($fJ/\mu m$)
3.9	5	0	1249	64	0.247	0.197
		1	1521	73	0.187	0.182
		2	1006	37	0.225	0.145
	3	1	128	103	1.63	0.134
		2	381	52	0.466	0.114
		3	296	71	0.629	0.119
	2	2	61	160	2.52	0.098
		3	193	65	0.741	0.091
	1	3	-	94	-	-
		4	-	169	-	-
25	5	0	1964	62	0.202	0.254
		1	2672	51	0.147	0.252
		2	2253	38	0.164	0.237
	3	1	674	96	0.415	0.179
		2	1215	57	0.244	0.189
		3	993	48	0.287	0.182
	2	2	708	140	0.346	0.157
		3	506	65	0.467	0.151
	1	3	451	87	0.449	0.13
		4	52	107	2.006	0.067
IRDS HP	12	-	924	75	0.78	0.47