Supplementary material for

Unravelling the atomic mechanisms of tetrahedral doping in chalcogenide glass for electrical switching materials

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Table S1. Summary of GeSe-based device performances using different dopants

Doping type	Material	Size	Selectivity	I_{off} (A)	V_{th} (V)	V_h (V)	Endurance	Thermal stability (℃)	V_{th} drift
None[1]	$Ge_{58}Se_{42}$	300	10^5	10^{-10}	3.5	1.7	10^9	N/A	N/A
Si[2]	$Ge_{42}Se_{58}$	200	~10^5	10^{-8}	2.5	N/A	10^5	320	Better
	$Ge_{37}Se_{50}Si_{13}$	200	10^4	>10^{-7}	2.0	N/A	>5×10^6	380	
N[3]	GeSe	300	N/A	$10^{-7.5}$	2.9	N/A	N/A	350	Better
	GeSeN	300	N/A	10^{-10}	4.5	N/A	N/A	450	
N[4]	GeSeN	50	10^5	2×10^{-9}	4.5	N/A	10^8	600	
C[3]	GeSe	300	N/A	$10^{-7.5}$	2.9	N/A	N/A	350	N/A
	GeSeC	300	N/A	$10^{-7.1}$	2.2	N/A	N/A	>350	
As[5]	GeAsSe	30	N/A	~10^{-10}	3.5	1.4	~10^{10}	450	Better
B[6]	GeSe	N/A	N/A	N/A	N/A	N/A	N/A	350	N/A
	GeSeB	6000	10^3	10^{-8}	1.5	N/A	N/A	330	
Sb[7]	$Ge_{60}Se_{40}$	N/A	N/A	N/A	3.24	2.2	N/A	420	Worse
	$GeSeSb_{22.5}$	N/A	10^5	N/A	2.16	0.8	N/A	>350	
Bi[8]	$Ge_{50}Se_{50}$	5000	10^6	N/A	7	N/A	N/A	400	N/A
	$GeSeBi_{9.5}$	5000	10^3	N/A	3	N/A	N/A	210	
Sn[9]	Ge56Se44	8000	N/A	N/A	3	1	N/A	~ 350	N/A
	GeSeSn	8000	N/A	N/A	<3	N/A	N/A	230	

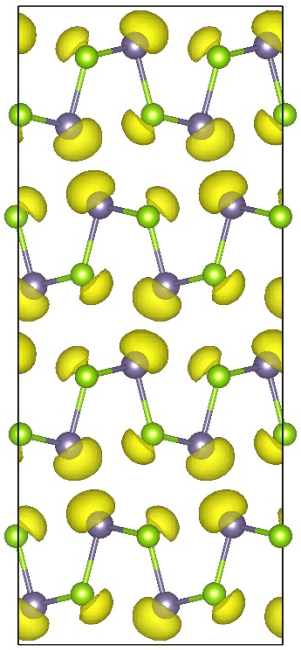

Fig. S1. The distribution of electron localized function (ELF) of crystal GeSe with an isovalue of 0.85, in which only shows the LP electrons located at the opposite side of covalent bonds near Ge and Se atoms and no electron located near the bonding area.

Table. S2 The statistic of Ge-Ge bonds per step at different quenching rates for a-GeSe and a-GeSiSe

	30 K/ps	20 K/ps	10 K/ps
a-GeSe	46.43	45.46	48.46
a-GeSiSe	88.93	87.59	91.65

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