The investigation of Na-related defects in $Cu_2ZnSnSe_4$

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Table S1 Convergence test of cut-off energy (take full relaxation of Na_{Zn} as an example).

E_{cutoff} (eV)	E_{tot} (eV)	Lattice constant (Å)		Average bond length (Å)		
		a	c	Cu-Se	Sn-Se	Zn-Se
370	-238.835	5.775	11.591	2.435	2.625	2.500
390	-283.826	5.775	11.593	2.435	2.625	2.500
410	-283.820	5.777	11.597	2.436	2.626	2.501

Fig. S2. Migration path of Na in $Cu_2ZnSnSe_4$ 1) Na_i-->Na_i 2)Na_i-->V_{Cu} 3) Na_{Cu}-->V_{Cu} 4)Na_{Zn}-->V_{Cu}.

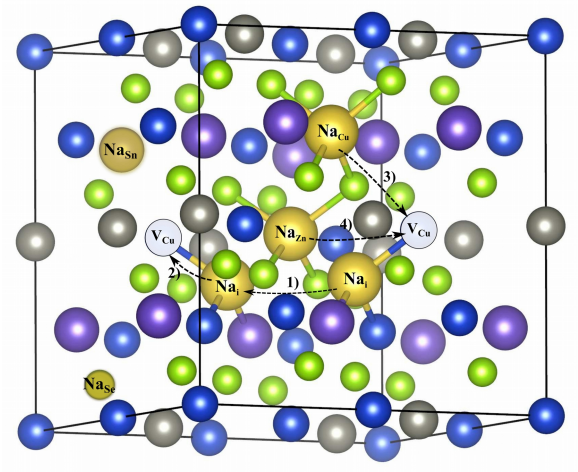

Fig. S1. The local density of states (LDOS) of NaCu, NaZn corresponding to the four nearest neighbor atoms around the substitutional Na with all the possible charge states in a 64-atom supercell using HSE06 functional. The energy is given referenced to the Fermi level.