Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Investigation of Sodium-ion Transport Mechanism and Elastic Properties of Double Anti-perovskite $Na_3S_{0.5}O_{0.5}I$

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Table S1. Relative energies of different conformations of $Na_3S_{0.5}O_{0.5}I$.

Conformation	Relative energy (eV)
1	0.13
2	0.17
3	0.09
4	0.14
5	**0.00**

Table S2. E_{defect} of different intrinsic defect configurations of Na_3OI and $Na_3S_{0.5}O_{0.5}I$.

Material	Defect	E_{defect} (eV)		
		NN	2NN	3NN
Na_3OI	NaI Schottky	**1.65**	1.70	1.81
	Na_2O Schottky	1.81	**1.72**	3.58
	Na Frenkel	**2.56**	2.62	2.71
$Na_3S_{0.5}O_{0.5}I$	NaI Schottky	**1.28**	1.29	1.40
	Na_2O Schottky	**2.33**	2.42	4.44
	Na_2S Schottky	**1.15**	1.16	to NN
	Na Frenkel	**1.63**	1.75	1.76

Table S3. $E_{solution}$ of different doping configurations of Na_3OI and $Na_3S_{0.5}O_{0.5}I$.

Material	Defect	$E_{solution}$ (eV)				
		NN	2NN	3NN	4NN	5NN
Na_3OI	$Mg_{Na}^{\bullet}$	-1.34	**-1.58**	-1.11	-1.04	-1.05
	$Ca_{Na}^{\bullet}$	**-0.46**	-0.43	-0.21	-0.15	-0.17
	$Sr_{Na}^{\bullet}$	**0.04**	0.26	0.34	0.41	0.37

	$Ba_{Na}^{\bullet}$	**0.72**	1.15	1.15	1.22	1.15
$Na_3S_{0.5}O_{0.5}I$	$Mg_{Na}^{\bullet}$	-0.98	**-1.17**	-0.68	-0.67	-0.67
	$Ca_{Na}^{\bullet}$	-0.37	**-0.45**	-0.06	-0.06	-0.06
	$Sr_{Na}^{\bullet}$	-0.05	**-0.08**	0.30	0.31	0.27
	$Ba_{Na}^{\bullet}$	**0.26**	0.43	0.88	0.89	0.81

Table S4. E_b along different paths in the lowest energy doping configuration.

Material	Defect	E_b (eV)				
		Path 1	Path 2	Path 3	Path 4	Path 5
Na_3OI	$Mg_{Na}^{\bullet}$	0.58	0.63			
	$Ca_{Na}^{\bullet}$	0.62	0.50	0.56	0.66	0.57
	$Sr_{Na}^{\bullet}$	0.67	0.63	0.55	0.68	0.59
	$Ba_{Na}^{\bullet}$	0.76	0.77	0.56	0.75	0.64
$Na_3S_{0.5}O_{0.5}I$	$Mg_{Na}^{\bullet}$	0.32	0.60			
	$Ca_{Na}^{\bullet}$	0.28	0.65			
	$Sr_{Na}^{\bullet}$	0.21	0.64			
	$Ba_{Na}^{\bullet}$	0.92	0.28	0.55	0.49	0.75

Table S5. Ionic conductivities and activation energies of $Na_3S_{0.5}O_{0.5}I$, Na_3OI and other Na^+ conducting materials.

Material	Ionic conductivity	activation energy	References
$Na_{10}GeP_2S_{12}$	4.7×10^{-3} S cm^{-1}	0.2	[58]

$Na_{3+x}Si_xP_{1-x}S_4$	1.66× 10^{-3} S cm^{-1}	0.24	[59]
$Na_{3+x}Ge_xP_{1-x}S_4$	5.4× 10^{-4} S cm^{-1}	0.28	[59]
$Na_{3+x}Sn_xP_{1-x}S_4$	1.07× 10^{-2} S cm^{-1}	0.17	[59]
$Na_{3.1}Zr_{1.95}Mg_{0.05}Si_2PO_{12}$	3.5 ×10^{-3} S cm^{-1}	0.25	[60]
$Na_{11}Sn_2PS_{12}$	1.4× 10^{-3} S cm^{-1}	0.25	[61]
$Na_{10}SnP_2S_{12}$	4× 10^{-4} S cm^{-1}	0.356	[62]
$Na_3S_{0.5}O_{0.5}I$	1.2 × 10^{-3} S cm^{-1}	0.20	Our work
Na_3OI	1.5 × 10^{-6} S cm^{-1}	0.42	Our work

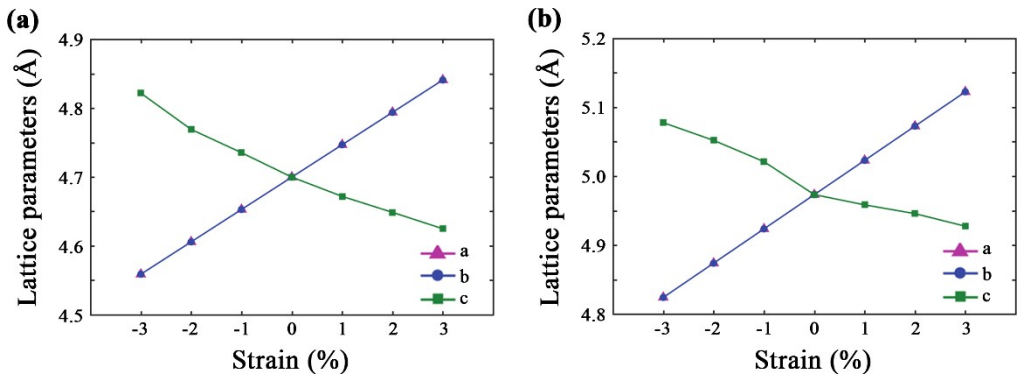

Fig. S1. Structural parameters of (a) Na_3OI and (b) $Na_3S_{0.5}O_{0.5}I$ under various biaxial strains in the a-b plane.