Computational Evaluation of Na_3SbX_3 (X =S, Se) for resistive switching memory devices for Neuromorphic Computing applications

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Abstract

- The structural, mechanical, and optoelectronic properties of Na_3SbX_4 (X = S, Se) chalcogens are investigated using Full Potential Linearly Augmented Plane Wave (FP-LAPW) based on Density Functional Theory (DFT)
- Perdew Burke Ernzerhof-Generalized Gradient Approximation (PBE-GGA) is used for structural optimization, while PBE-SOL and WC-GGA is employed for electronic band structure and optical response analysis.
- Structure is found to be stable, appropriate for synthesis and device fabrication.
- Both materials possess mechanical stability under effect of pressure.
- The compounds are found to be semiconductors, with a decreasing bandgap as Se is replaced with S ion.
- Optical properties align with the electronic band structure.
- Se base material possess increased absorption and reduced energy loss, offering tunability of resistance between High Resistance State (HRS) and Low Resistance State (LRS)

Computational methodology

- Ab-initio calculations with framework of DFT using VASP simulation tool
- Supercell of 2×2×2 was used to estimate structural, mechanic and optoelectronic properties
- Ionic and Lattice relaxation was done to find fully optimized structure
- Hybrid functionals were used to compare results and explore more properties

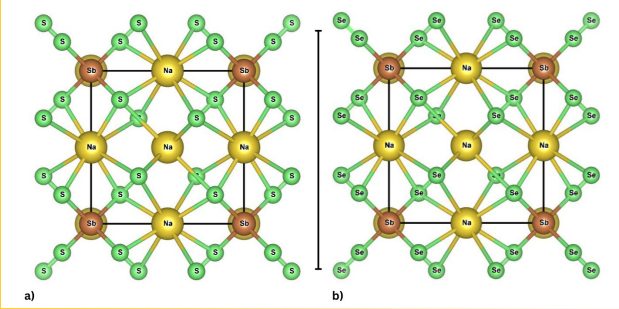

Figure. 1 Optimized crystal structure of a) Na_3SbS_4 and b) Na_3SbSe_4

Material	Na_3SbS_4	Na_3SbSe_4
Lattice parameter (Å)	7.264	7.4618
Density (g/cm^3)	2.76	2.44
Ground state volume ($Å^3$)	383.33	415.47
Formation Energy (KeV/atom)	-0.104	-0.102
Tolerance factor	0.822	0.816

Table. 1 The extracted optimized lattice parameters of Na_3SbX_4 (X=S, Se)

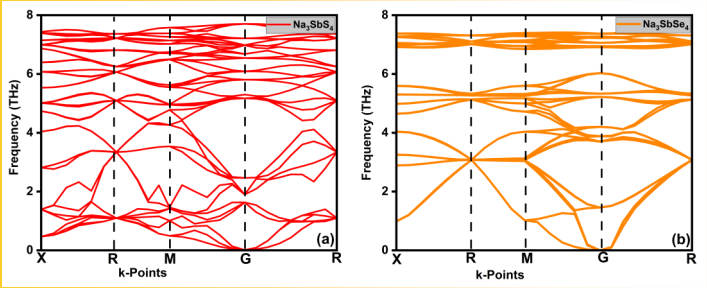

Figure. 2 Computed phonon modes of Na_3SbX_4 (X=S, Se) chalcogens

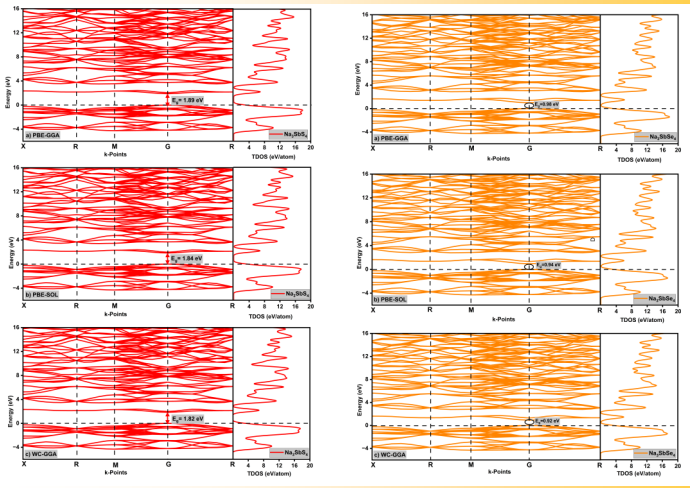

Figure. 3 Calculated electronic band structures and total density of states (TDOS) for Na_3SbX_4 (X= S, Se)

Material	PBE-GGA (eV)	PBE-SOL (eV)	WC-GGA (eV)
Na_3SbS_4	1.89	1.84	1.82
Na_3SbSe_4	0.98	0.94	0.92

Table. 2 The summary of energy band gap calculated through different potentials for Na_3SbX_4 (X= S, Se)

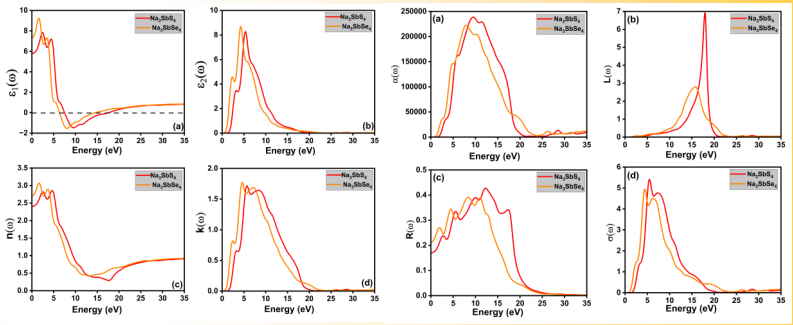

Figure.4 Calculated optical properties of Na_3SbX_4 (X= S, Se)

Material	Na_3SbS_4	Na_3SbSe_4
Bulk modulus (B)	24.06	28.99
Young's modulus (Y)	26.71	42.39
Shear modulus (G)	10.16	16.92
Pough Ratio (B/G)	2.36	1.71
Poisson Ratio	0.31	0.26

Table. 3 The extracted optimized lattice parameters of Na_3SbX_4 (X=S, Se)

Conclusion

- Both materials possesses a stable structure
- Both materials are mechanically and thermally stable
- Band gap decreases on replacement of Se ion with S ion
- Electronic and Optical properties align with each other
- Na_3SbSe_4 possess less energy loss function and better absorption upon incident light