Post-Christmas Update

Ben Goldmann

February 9, 2021

Initial vs Refitted

Buckingham potentials

Na-O	1226.84 0.307 0	1225.11 0.307 0
Na-Cl	2314.70 0.290 0	2292.53 0.290 0

Literature search

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SHORT COMMUNICATION

INTERNATIONAL JOURNAL OF ENERGY RESEARCH WILEY

The structural stability, lattice dynamics, electronic, thermophysical, and mechanical properties of the inverse perovskites A_3OX: A comparative first-principles study

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Summary

We present a comparative study on the structural, electronic, elastic, and thermoelectric properties of the cubic inverse-perovskites A_3OX (where A = Li, Na, K and X = Cl, Br, I) by density functional theory (DFT). The cohesive, formation, and elastic properties analysis indicates that all studied materials are chemically, thermodynamically, and mechanically stable. Electronic properties reveal that all the inverse A_3OX perovskite are direct bandgap semiconductors except Li_3OCl and Li_3OBr with ionic nature which is confirmed by electron localization function (ELF) analysis. We have also calculated Debye temperature (Θ_D) and Grüneisen parameter (γ) to determine the lattice thermal conductivity for all the A_3OX materials. Furthermore, thermoelectric (TE) properties are explored by calculating the Seebeck coefficient (S), electronic thermal conductivity, power factor (PF), electrical conductivity (σ/τ), lattice thermal conductivity, and ZT value. Our investigated A_3OX inverse-perovskites provide a fertile base that can improve the overall TE performance for TE applications and green energy production.

KEYWORDS
antiperovskite, formation energy, mechanical properties, phonon, p-type semiconductors, structural properties, thermoelectric properties

Sattar et al. (2020)

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Ab initio study of electronic structure, elastic and optical properties of anti-perovskite type alkali metal oxyhalides

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ABSTRACT

We report the structural, elastic, electronic, and optical properties of antiperovskite alkali metal oxyhalides Na_3OCl, Na_3OBr, and K_3OBr using two different density functional methods within generalized gradient approximation (GGA). Plane wave pseudo potential (PW-PP) method has been used to calculate the ground state structural and elastic properties while the electronic structure and optical properties are calculated explicitly using full potential-linearized augmented plane wave (FP-LAPW) method. The calculated ground state properties of the investigated compounds agree quite well with the available experimental data. The predicted elastic constants using both PW-PP and FP-LAPW methods are in good accord with each other and show that the materials are mechanically stable. The low values of the elastic moduli indicate that these materials are soft in nature. The bulk properties such as shear moduli, Young's moduli, and Poisson's ratio are derived from the calculated elastic constants. Tran–Blaha modified Becke–Johnson (TB–mBJ) potential improves the band gaps over GGA and Engel-Vosko GGA. The computed TB–mBJ electronic band structure reveals that these materials are direct band gap insulators. The complex dielectric function of the metal oxyhalide compounds have been calculated and the observed prominent peaks are analyzed through the TB–mBJ electronic structures. By using the knowledge of complex dielectric function other important optical properties including absorption, reflectivity, refractive index and loss function have been obtained as a function of energy.

Ramana et al. (2013)

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Elastic Properties of Alkali Superionic Conductor Electrolytes from First Principles Calculations

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In this work, we present a comprehensive investigation of the elastic properties (the full elastic tensor, bulk, shear and Young's moduli, and Poisson's ratio) of 23 well-known ceramic alkali superionic conductor electrolytes (SICEs) using first principles calculations. We find that the computed elastic moduli are in good agreement with experimental data (wherever available) and chemical bonding nature. The anion species and structural framework have a significant influence on the elastic properties, and the relative elastic moduli of the various classes of SICEs follow the order thiophosphate < antiperovskite < phosphate < NASICON < garnet < perovskite. Within the same framework structure, we observe that Na SICEs are softer than their Li analogs. We discuss the implications of these findings in the context of fabrication, battery operation, and enabling a Li metal anode. The data computed in this work will also serve as a useful reference for future experiments as well as theoretical modeling of SICEs for rechargeable alkali-ion batteries.

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Deng et al. (2016)

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RESEARCH ARTICLE

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Electronic structure, thermomechanical and phonon properties of inverse perovskite oxide (Na_3OCl): An ab initio study

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Summary

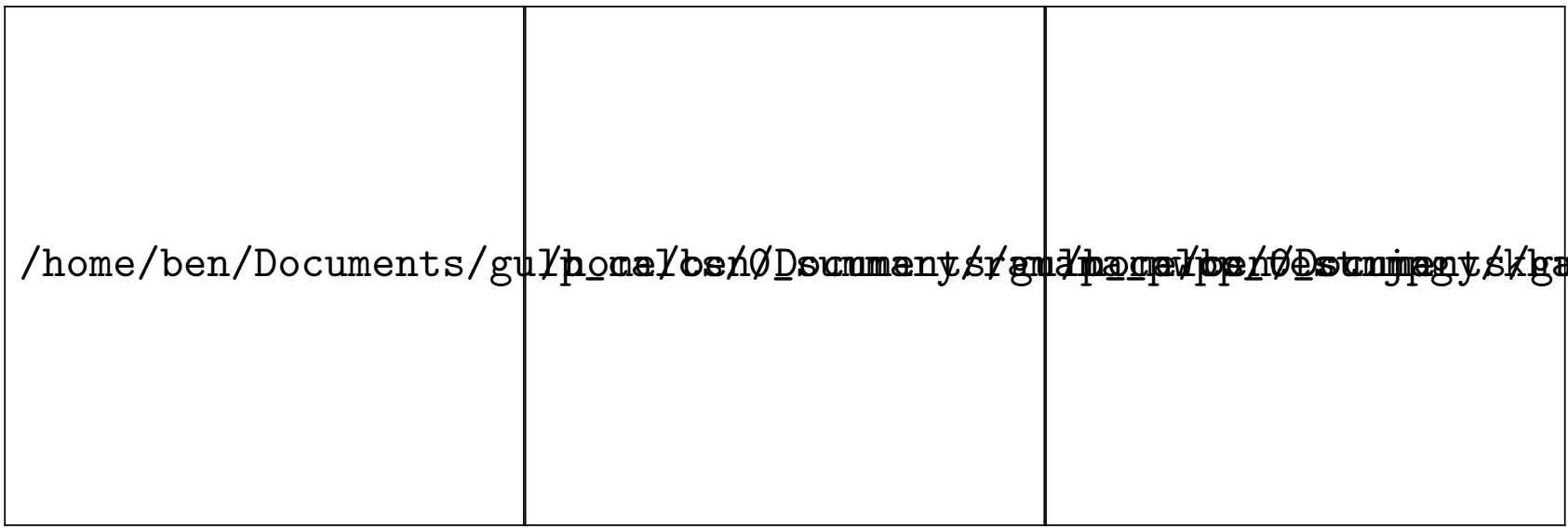
Within first principles calculations, the electronic structure, thermodynamic, mechanical stability, magnetism, and phonon properties of the inverse perovskite (Na_3OCl) have been summed up. The Birch-Murnaghan derived lattice constant and bond-lengths are identical, when compared to the experimental data. A direct energy gap of 2.18 eV observed from the band structure reveals the semiconducting nature of the present oxide. Also, the application of strain on electronic properties predicts the decrease in bandgap with respect to compressive strain and vice versa. The constituent nonmagnetic atoms in its crystal propose the total magnetic moment to be zero and the same is supported by susceptibility data. In addition to the negative Cauchy's pressure, the small bulk modulus compared to Young's modulus determined from elastic constants, possibly claims it as a brittle material. Also, the temperature dependent Gruneisen parameter (1.58) and Debye temperature (382.27 K) are determined to reveal the lattice thermal conductivity (κ = 6.48 W/mK) at room temperature.

KEYWORDS
electronic structure, mechanical strength, phonon properties, structural properties, thermal conductivity

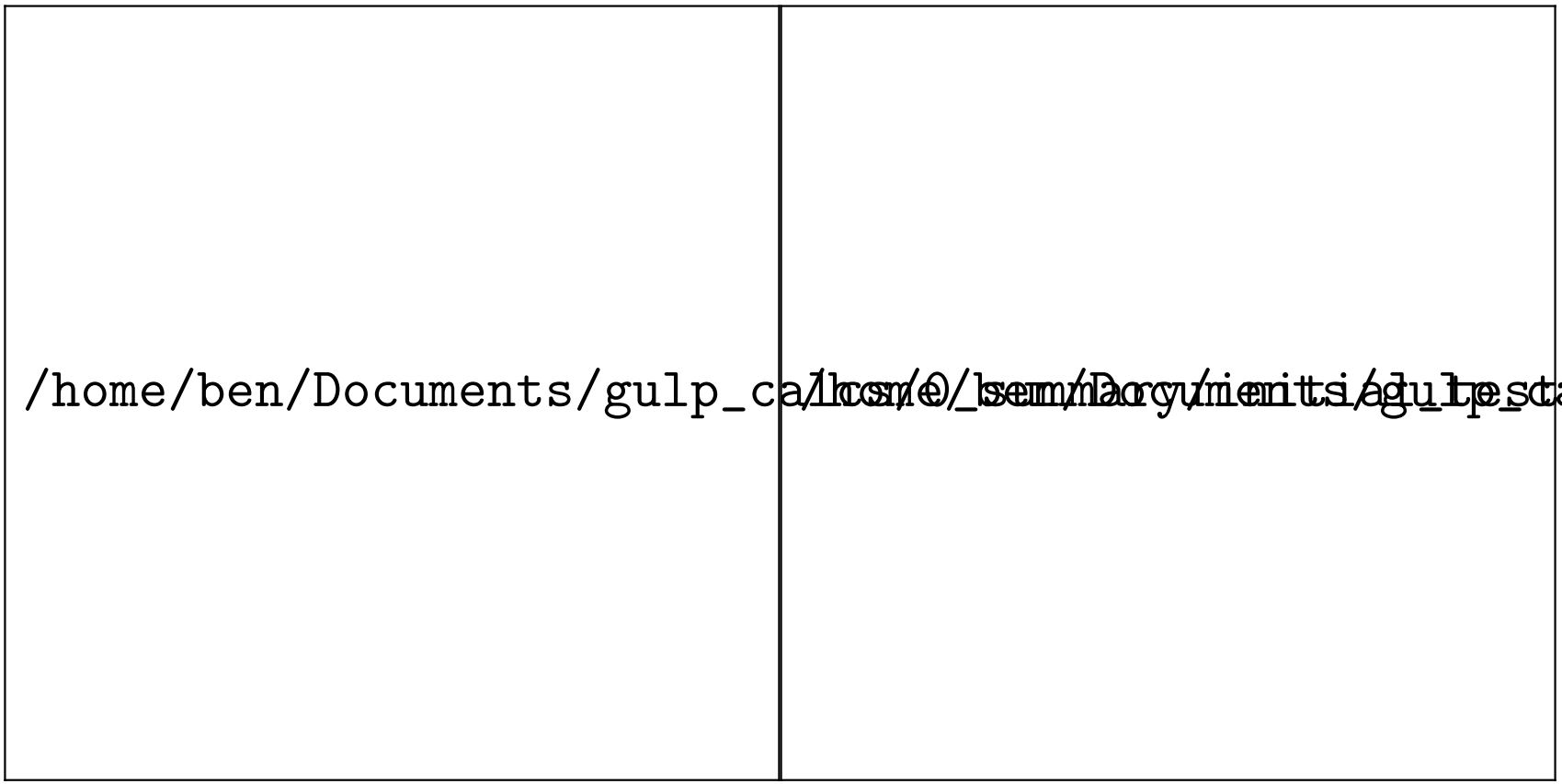
Khandy et al. (2020)

Data used and potentials calculated

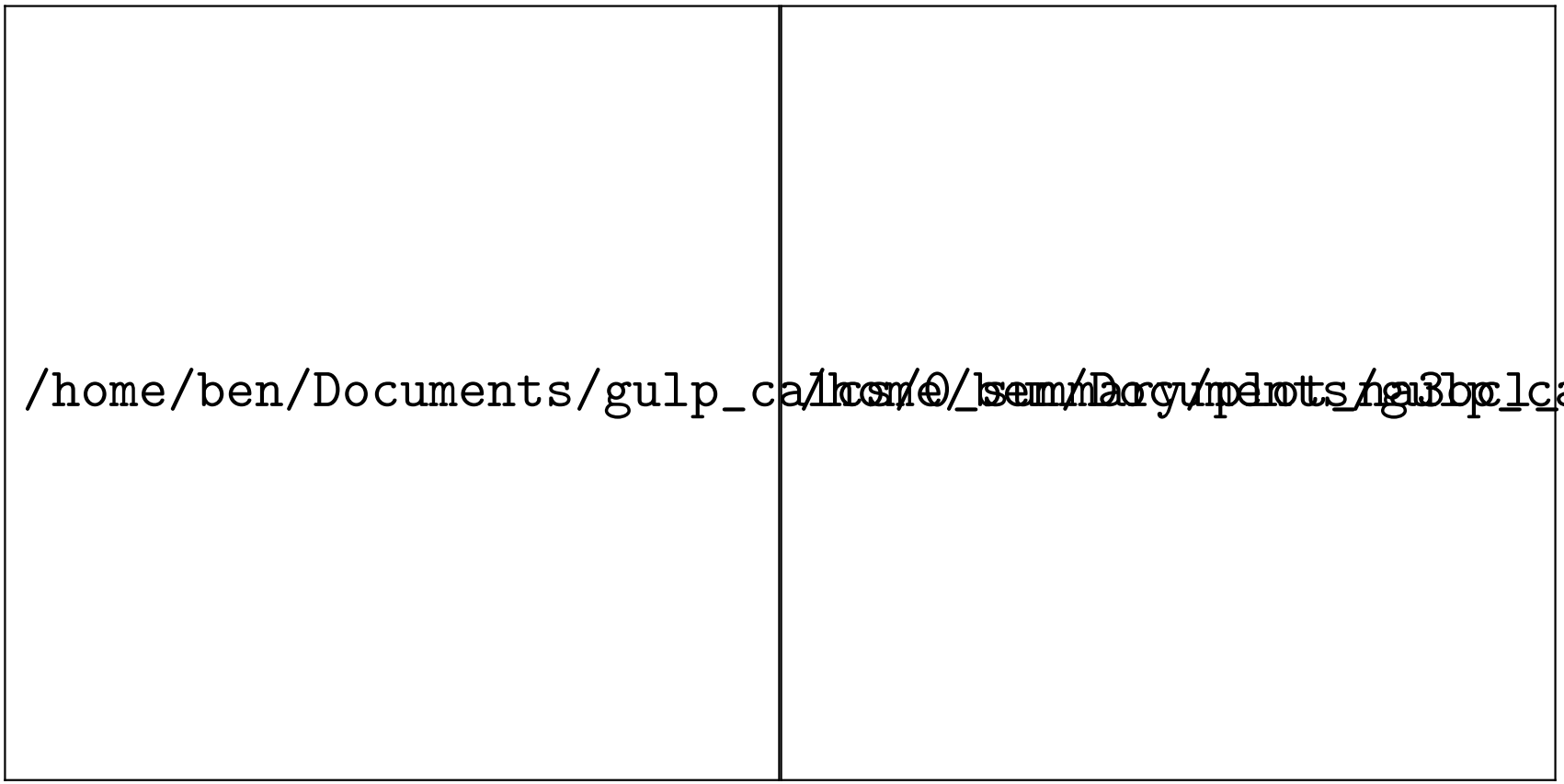
Paper	Model	Bulk, GPa	Shear, GPa	Na-O Buckingham	Na-Cl Buckingham	Variation
Original	N/A	N/A	N/A	1226.84 0.307 0	2314.70 0.290 0	N/A
Ramana2013	FP-LAPW GGA	32.5	21.9	322.01 0.388 0	1727.87 0.297 0	3.55
Ramana2013	PW-PP GGA	34.2	22.9	369.22 0.376 0	1775.12 0.300 0	0.58
Deng2016	PAW GGA	36.4	24.6	1042.96 0.310 0	1591.38 0.288 0	20.35
Khandy2020	FP-LAPW GGA	33.45	26.87	588.38 0.338 0	1170.41 0.315 0	0.04
Sattar2020	FP-LAPW GGA	32.53	25.42	477.56 0.354 0	1270.12 0.309 0	0.61



Comparison of Initial and Khandy potentials



Comparison of Initial and Khandy potentials



Calculations using potentials derived from Khandy2020

Parameter	Calc.	Comp. GGA	Comp. LDA	Comp. GULP	Experimental
lattice parameter, $\AA$	4.41	4.54[1], 4.538[2], 4.53[3], 4.543[4], 4.514[4], 4.541[5]	4.382[2], 4.381[4], 4.31[6]	4.501[7]	4.504[8], 4.496[9], 4.500[10], 4.4908[11]
Na Frenkel, eV	2.58	1.94[1], 2.45[7]			
NaCl Schottky, eV	1.88	1.28[1], 1.75[7]			
Na_2O Schottky, ev	5.14	2.52[1]			
Na_3OCl Schottky, ev	6.74	6.10[7]			
Na vacancy migration, eV	0.46	0.61[1], 0.428[11], 0.29[8], 0.29[7]			0.63[11], 1.04[8]

Review of results

- Concern over slightly off lattice parameter
- Discussion with Ben and Lucy
- They suggested that while the results may look good, they might not be accurate
- They proposed trying to fit the potentials using Lucy's code
- This involves thermally distorting the initial structure via AIMD, taking snapshots,, doing single-point calculations on the snapshots and fitting the potentials to them

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