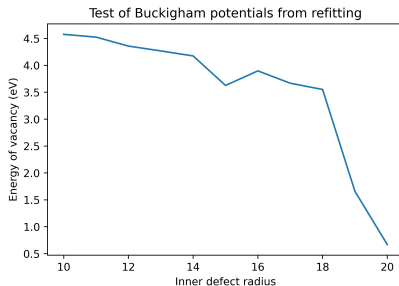
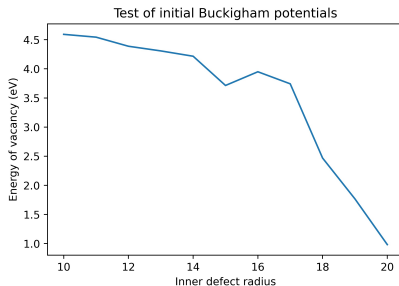


# Post-Christmas Update

Ben Goldmann

January 5, 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

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SHORT COMMUNICATION



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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Funding Information  
United Arab Emirates University

Summary

We present a comparative study on the structural, electronic, elastic, and thermodynamic 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, vibrational, and elastic properties analysis indicates that all studied materials are chemically, thermodynamically, and mechanically stable. Electronic properties reveal that all the inverse  $A_3OX$  perovskites 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 ( $\Theta_D$ ) and Grüneisen parameter ( $\gamma$ ) to determine the lattice thermal conductivity for all the  $A_3OX$  materials. Furthermore, thermodynamic (TE) properties are explored by calculating the Seebeck coefficient ( $S$ ), electronic thermal conductivity, power factor (PF), electrical conductivity ( $\sigma$ ), 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

inverse-perovskite, formation energy, mechanical properties, phonon,  $p$ -type semiconductors, structural properties, thermodynamic properties

Sattar et al. (2020)



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

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ABSTRACT

We report structural, elastic, electronic, and optical properties of antiperovskite alkali metal oxyhalides  $Na_3XCl$ ,  $Na_3XBr$ , and  $K_3XBr$  using two different density functional methods: either generalized gradient approximation (GGA) or PBEsol method. The calculated elastic constants are used to calculate the ground state structural and elastic properties while the electronic and optical properties are investigated by employing the full potential linearized augmented plane wave method. The calculated ground state properties of the investigated compounds agree well with the available experimental data. The predicted elastic constants using both PBEsol and GGA methods are in good accord with each other and show that the materials are mechanically stable. The low values of the elastic modulus indicate that these materials are soft in nature. The bulk properties such as elastic modulus, Young's modulus, and Poisson's ratio are derived from the calculated elastic constants. The  $Na_3XBr$  exhibits better electronic band structure results than the other materials are direct band gap semiconductors. The complete dielectric function of the total oxyhalide compounds have been calculated and the observed prominent peaks are analyzed through the 10-ns model approximation. 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.

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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 of the full ionic crystal, the alkali and the superionic phases of the alkali superionic conductor electrolytes (SECs) using first principles calculations. We find that the computed elastic moduli are in good agreement with experimental data and theoretical banding nature. The atom species and structural framework have a significant influence on the elastic properties, and the relative elastic moduli of the various classes of SECs follow the order: fluorides > oxides > nitrides > sulfides > phosphides > arsenides > antimonides > tellurides. Within the same framework structure, we observe that Na SECs are softer than Li analogs. We discuss the implications of these findings on the context of laboratory synthesis operation, and making a useful guide. The data computed in this work will also serve as a useful reference for future experiments as well as theoretical modeling of SECs for rechargeable solid ion batteries. © 2015 The Electrochemical Society. [DOI: 10.1149/1.5204444] All rights reserved.

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Deng et al. (2016)

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RESEARCH ARTICLE



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

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Mathias Gogolin<sup>1,5</sup> | Aurangzeb K. Hafez<sup>4</sup> | Azher M. Siddiqui<sup>2</sup>

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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 examined up to the Birch-Murnaghan derived bulk 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 possess the total magnetic moment to be zero and the state 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 Grüneisen parameter (1.59) and Debye temperature (362.2 K) are determined to reveal the lattice thermal conductivity ( $\kappa \approx 0.46$  W/mK) at room temperature.

KEYWORDS

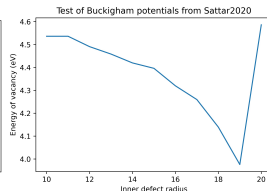
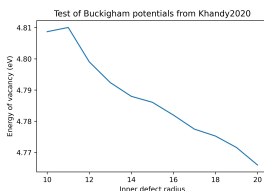
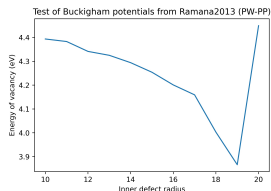
electronic structure, mechanical strength, phonon properties, structural properties, thermal conductivity

Khandy et al. (2020)

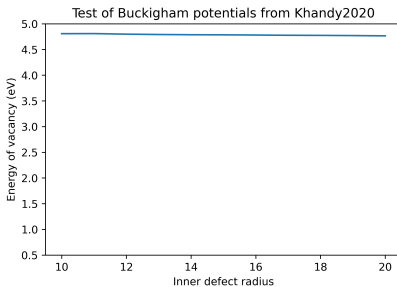
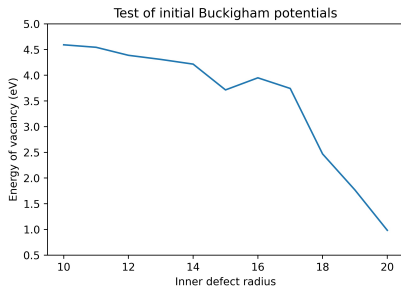
Ramana et al. (2013)

# Data used and potentials calculated

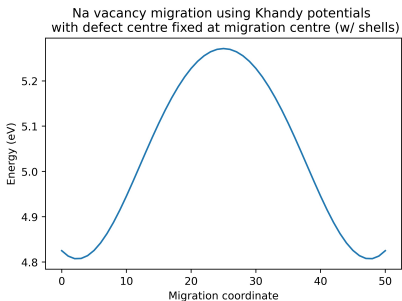
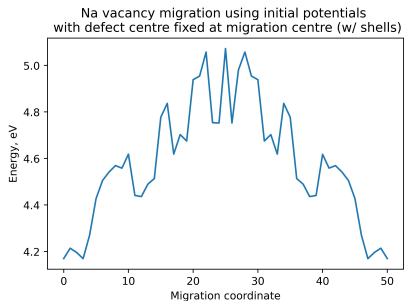
Paper	Model	Bulk, GPa	Shear, GPa	Na-O Buckingham	Na-Cl Buckingham	Variation
Original	N/A	N/A	N/A	1226.84 0.307 0	2314.70 0.290 0	N/A
Ramana2013	FP-LAPW GGA	32.5	21.9	322.01 0.388 0	1727.87 0.297 0	3.55
Ramana2013	PW-PP GGA	34.2	22.9	369.22 0.376 0	1775.12 0.300 0	0.58
Deng2016	PAW GGA	36.4	24.6	1042.96 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

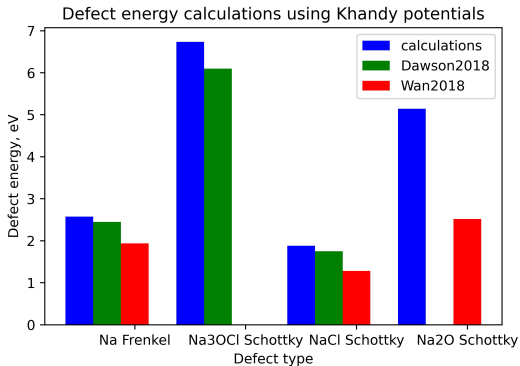


# Comparison of Initial and Khandy potentials



# Calculations using potentials derived from Khandy2020

Parameter	Calc.	Comp. GGA	Comp. LDA	Comp. GULP	Experimental
lattice parameter, Å	4.41	4.54 <sup>1</sup> , 4.538 <sup>2</sup> , 4.53 <sup>3</sup> , 4.543 <sup>4</sup> , 4.514 <sup>4</sup> , 4.541 <sup>5</sup>	4.382 <sup>2</sup> , 4.381 <sup>4</sup> , 4.31 <sup>6</sup>	4.501 <sup>7</sup>	4.504 <sup>8</sup> , 4.496 <sup>9</sup> , 4.500 <sup>10</sup> , 4.4908 <sup>11</sup>
Na Frenkel, eV	2.58	1.94 <sup>1</sup> , 2.45 <sup>7</sup>			
NaCl Schottky, eV	1.88	1.28 <sup>1</sup> , 1.75 <sup>7</sup>			
Na <sub>2</sub> O Schottky, eV	5.14	2.52 <sup>1</sup>			
Na <sub>3</sub> OCl Schottky, eV	6.74	6.10 <sup>7</sup>			
Na vacancy migration, eV	0.46	0.61 <sup>1</sup> , 0.426 <sup>11</sup> , 0.29 <sup>8</sup>			0.63 <sup>11</sup> , 1.04 <sup>8</sup>



# Review of results

- ▶ 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 (involving fitting to DFT)



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