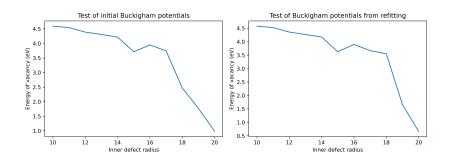
Post-Christmas Update

Ben Goldmann

January 11, 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

het 24 Fare 3031 | Reviset 19 September 3031 | Accepted 38 September 3031 SHORT COMMUNICATION



The structural stability, lattice dynamics, electronic, thermophysical, and mechanical properties of the inverse perovskites A3OX: A comparative first-principles study

Muhammad A. Sattar | Mehreen Javed | Maamar Benkraouda | Noureddine Amrane

Correspondence Nounddine Amrane, Physics Department College of Science, United Arab Emirate Funding information

moelectric properties of the cubic inverse-perovskites AsOX (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 A₂OX perovskite are direct bandgap semiconductors escept Li-OCI and Li-OBr with ionic nature which is confirmed by electron localization function (ELP) analysis. We have also calculated Delive temperature (Θ_D) and Grilneisen parameter (y) to determine the lattice thermal conductivity for all the A₂OX materials. Purthermore, thermoelectric (TE) properties are explored by calculating the Seebeck coefficient (S), electronic thermal conductivity, nower factor (PF), electrical conductivity (e/v). lattice thermal conductivity, and ZT value. Our investigated A₂OX inverseperovskites provide a fertile base that can improve the overall TE performance for TE applications and green energy production.

We present a communitive study on the structural, electronic, elastic, and then

Sattar et al. (2020)



Solid State Sciences



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

1. Ramanna*, N. Vedukondalu*, K. Ramesh Babu*, G. Vaitheeswaran* "School of Physics, University of Hydrodod, Prof. C. R. Rea Road, Hydrodod 200 Rei, Andhro Pradint, India
"Advanced Central of Research in High Energy Hearins's (HURBERS, University of Molecular, Prod. C. R. Rea Read, Hydrodod 200 Rei, Andhro Pradint, India

Accepted 12 March 2913 Acadable online 26 Namb 2013

dislocatic function other important options proposes monetage.

and loss function have been obtained as a function of energy.

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Ramana et al. (2013)

Journal of The Electrochemical Society, 163 (2) A67-A74 (2016)

Elastic Properties of Alkali Superionic Conductor Electrolytes from First Principles Calculations Zhi Deng, Zhenbin Wang, Jek-Heng Chu, Jian Luo, and Shrue Ping Ong**

Department of NanoEngineering, University of California San Diego, La Jolia, California 92993-8488, USA and Patients' ratio of 23 with constraint of the properties of the patients of the state of the patients of th

Manuscript submitted August 51, 2015; revised manuscript received October 12, 2015. Published Nevember 5, 2015

Deng et al. (2016)

ENERGY RESEARCH WILEY

Electronic structure, thermomechanical and phonon properties of inverse perovskite oxide (Na₃OCI):

Shakeel Ahmad Khandy¹ | Ishtihadah Islam² | Amel Laref³ | Mathias Gogolin^{4,5} | Aurangzeb K. Hafiz⁶ | Azher M. Siddiqui²

'Department of Physics, Jamia Milia Department of Physics, College of

An ab initio study

MAPEX Copper for Magnish and Shaked A. Khandy, Department of

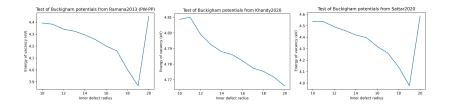
Funding information

Within first principles calculations, the electronic structure, thermodynamic, mechanical stability, magnetism, and phonon properties of the inverse persyskite (Na-OCI) 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 bundgap with respect to compressive strain and vice versa. The constituent nonnagnetic atoms in its crystal 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 (582.27 K) are determined to reveal the lattice thermal conductivity (e = 6.48 W/mK) at room

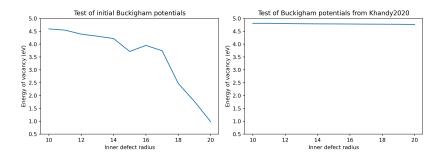
Khandy et al. (2020)

Data used and potentials calculated

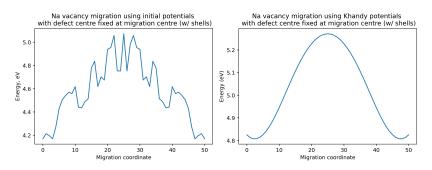
Paper	Model	Bulk, GPa	Shear, GPa	Na-O Buckingham	Na-Cl Buckingham	Variation
Original	N/A	N/A	N/A	1226.84 0.307 0	2314.70 0.290 0	N/A
Ramana2013	FP-LAPW GGA	32.5	21.9	322.01 0.388 0	1727.87 0.297 0	3.55
Ramana2013	PW-PP GGA	34.2	22.9	369.22 0.376 0	1775.12 0.300 0	0.58
Deng2016	PAW GGA	36.4	24.6	1042.96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

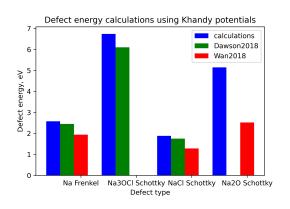


Comparison of Initial and Khandy potentials



Calculations using potentials derived from Khandy2020

Parameter	Calc.	Comp. GGA	Comp. LDA	Comp. GULP	Experimental
lattice parameter, A	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	4.5017	4.5048, 4.4969, 4.50010, 4.490811
Na Frenkel, eV	2.58	1.94 ¹ , 2.45 ⁷			
NaCl Schottky, eV	1.88	1.28 ¹ , 1.75 ⁷			
Na ₂ O Schottky, ev	5.14	2.52 ¹			
Na ₃ OCI Schottky, ev	6.74	6.107			
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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