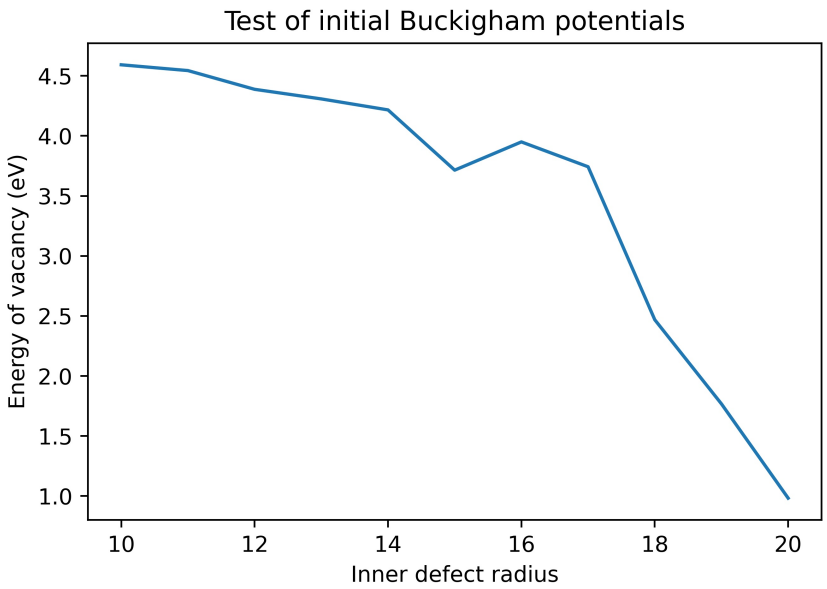
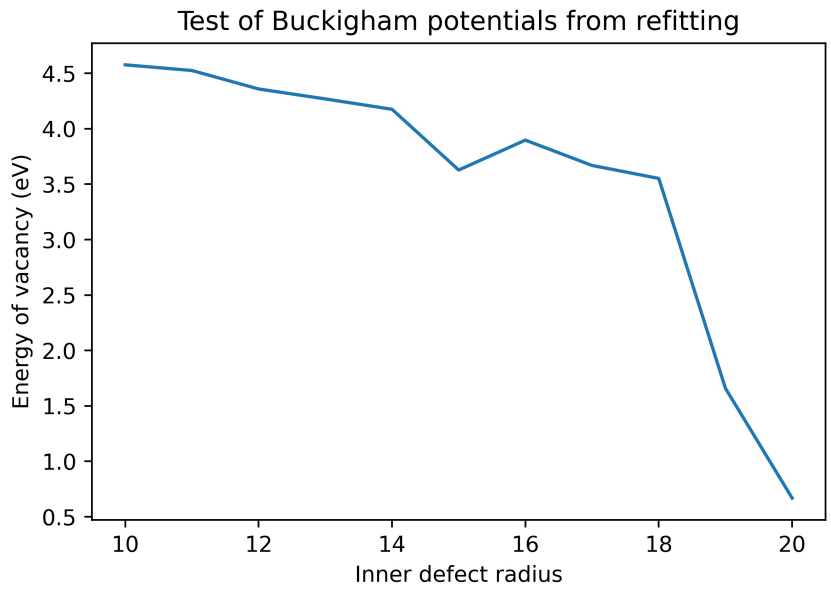
Post-Christmas Update

Ben Goldmann

January 2, 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

Journal of The Electrochemical Society, **163** (2) A67-A74 (2016)
0013-4651/2016/163(2)/A67/8/$33.00 © The Electrochemical Society

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 at 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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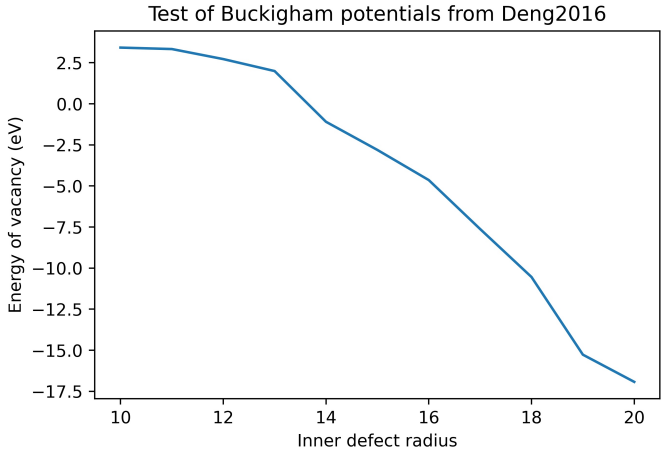
Summary
Within first principles calculations, the electronic structure, thermodynamic, mechanical stability, magnetism, and phonon properties of the inverse perovskite (Na_3OCl) have been summed up. The Birch-Murnaghan derived lattice constant and bond-lengths are identical, when compared to the experimental 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)

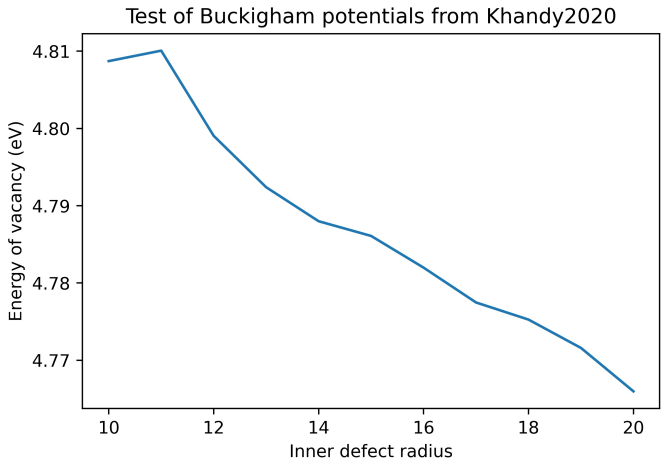
Data used and potentials calculated

1. Deng et al. (2016)
   - Bulk modulus: 36.4 GPa
   - Shear modulus: 24.6 GPa
   - Na-O: 1042.96 0.310 0 (vs 1226.84 0.307 0)
   - Na-Cl: 1591.38 0.288 0 (vs 2314.70 0.290 0)



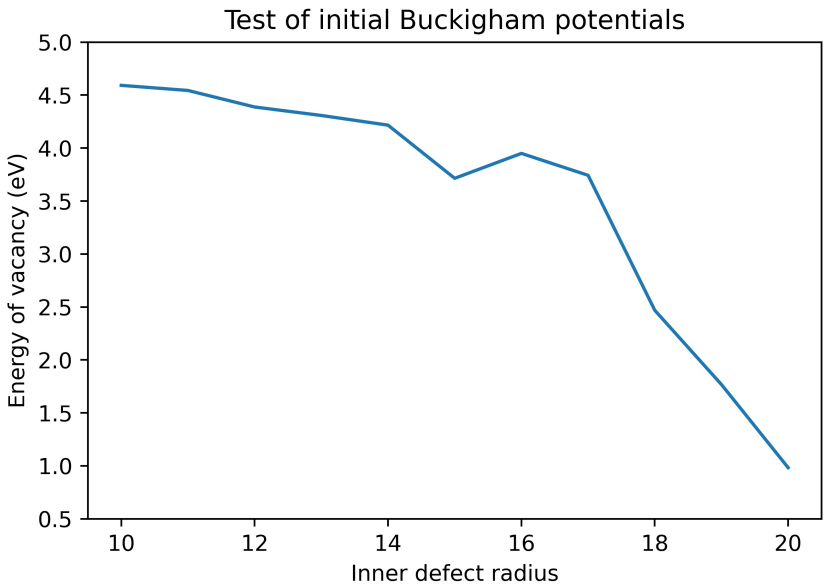
Deng2020

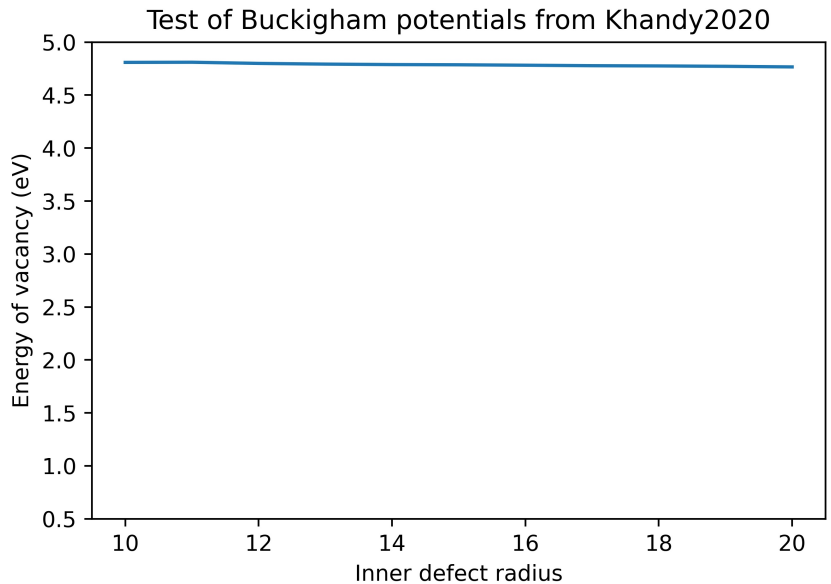
2. Khandy et al. (2020)
   - Bulk Modulus: 33.45 GPa
   - Shear modulus: 26.87 GPa
   - Na-O: 588.38 0.338 0 (vs 1226.84 0.307 0)
   - Na-Cl: 1170.41 0.315 0 (vs 2314.70 0.290 0)



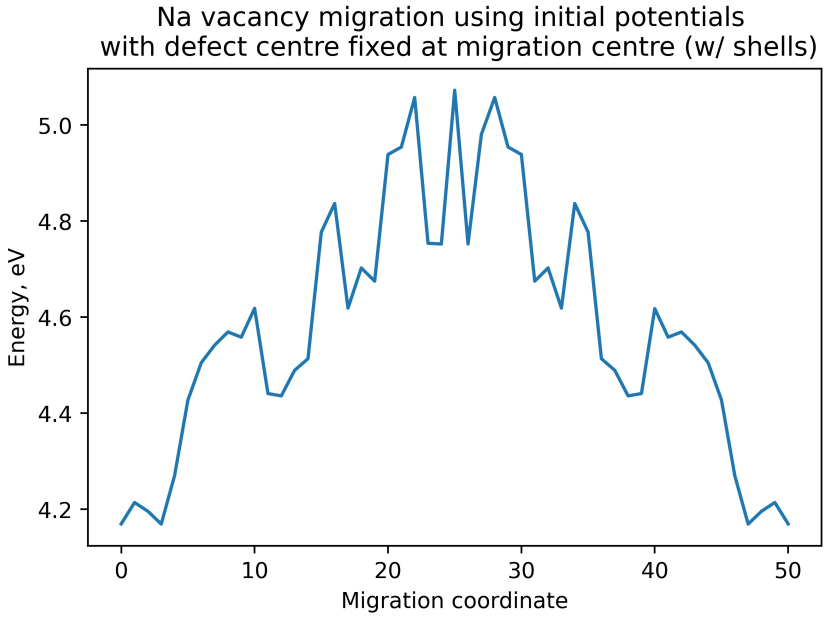
Khandy2020

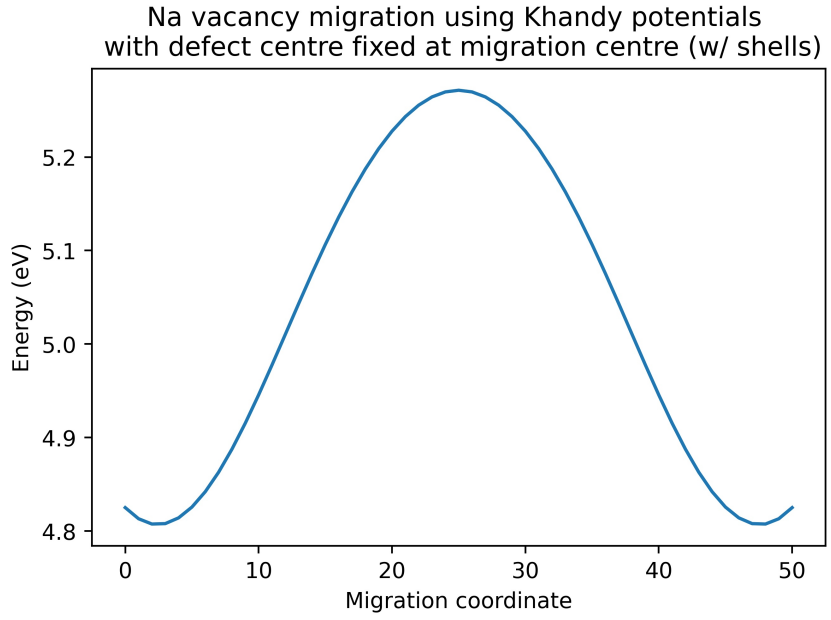
Comparison of Initial and Khandy





Comparison of Initial and Khandy 2





Calculations using Khandy potentials

Na vacancy defect energy: 4.78 eV
Na vacancy migration barrier: 0.46 eV
Na interstitial defect energy: -2.21 eV
O vacancy defect energy: 21.88 eV
O interstitial defect energy: -14.24 eV
Cl vacancy defect energy: 5.19 eV
Cl interstitial defect energy: -1.51 eV
Na3OCl Schottky defect energy: 6.74 eV
NaCl partial Schottky defect energy: 1.88 eV
Na2O partial Schottky defect energy: 5.14 eV
Na Frenkel defect energy: 2.58 eV
O Frenkel defect energy: 7.64 eV
Cl Frenkel defect energy: 3.68 eV
Lattice energy of Na3OCl (from calculations): -34.68 eV
Lattice energy of NaCl (from calculations): -8.09 eV
Lattice energy of Na2O (from calculations): -26.3 eV