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Slater Insulator Phase of X_2 ($X = \text{Na}, \text{Li}$) IrO_3 : First Principles Calculation

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ABSTRACT

In the present work, the structural, electronic and mechanical properties of Na_2IrO_3 and Li_2IrO_3 have been investigated by means of first principles calculations. The spin polarized generalized gradient approximation has been used for modeling exchange-correlation effects. The structural optimization of these compounds has been performed by using VASP-code, and the lattice parameters and magnetic moments have been calculated. From our calculation, it has been determined that $X_2\text{IrO}_3$ ($X = \text{Na}, \text{Li}$) compounds for both spin up and spin down states are indirect wide gap semiconductor in nature. Considering the spin states from the electronic band structure and density of the state (DOS) of the Na (Li) $_2\text{IrO}_3$ compounds, it has been identified that $E_g = 1.824$ (2.315) eV for spin up and $E_g = 1.558$ (2.019) eV for spin down. The second-order elastic constants have been calculated, and the other related quantities have also been estimated in the present work.

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1. Introduction

Recently, Slater insulators display the properties of metals at a sufficiently high temperature, they become insulators when cooled to a certain temperature (transition temperature) peculiar to the substance concerned. Correlated honeycomb transition metal oxides (TMOs) $X_2\text{IrO}_3$ ($X = \text{Li}, \text{Na}$) are the Slater insulator with the highest transition temperature and attracts large attention for being at the intersection of various physical phenomena that are in the focus of current research due to their potential relevance for future technological application as well as for fundamental questions [1–5]. The nd ($n = 3, 4$, and 5) TMO bring in a strong intra-atomic spin-orbit coupling (SOC) on top of the dominant interatomic spin-spin interactions seen in nd TMO [4–7]. Due to the electron-electron interactions and spin orbital coupling of Ir atoms, $X_2\text{IrO}_3$ compounds have attracted also great interest as a materials with an unusual phase of matter that can be formed by interacting quantum spins in certain magnetic materials (Kitaev model). The Kitaev model describes a 2-D quantum magnet with possible applications in quantum computing [8]. The ground state of the Kitaev model includes spin liquid

phases. Therefore, Kitaev quantum spin liquid (KQSL) is a topological phase of matter arising from the exactly solvable Hamiltonian of the nearest neighboring bond directional interactions between half integer spins in a honeycomb lattice [9]. The energy scales of SOC, Coulomb repulsion and band width resulting from nd TMO can become comparable with each other. This results in broad spectrum of quantum phases such as spin liquid, topological insulator and Mott insulator. It is debated whether the nature of the insulating phase in iridium oxides is a Mott type insulator or a Slater type insulator [1, 2]. Na_2IrO_3 compounds consist of alternating stacking of honeycomb NaIr_2O_6 layers separated by hexagonal Na_3 layers [10, 11]. Li_2IrO_3 structures can be derived from Li-ion battery cathode material LiCoO_2 by ordering Li and Ir ions [12]. The changes in the band topology crystal structure cause the magnetic and electronic structures of X_2IrO_3 compounds to change significantly. There are striking inconsistencies between theoretical and experimental observations regarding these compounds. Therefore, it appears that there is a characterization deficiency with regard to these compounds [13].

A lot of experimental and theoretical studies have been done on $\text{X}_2(\text{X} = \text{Na}, \text{Li})\text{IrO}_2$ compounds [10–15]. Some of these studies are summarized here. Vasdev et al. [14] studied in detail the physical, chemical and electronic properties of the surface of the Na_2IrO_3 compound using probe microscopy in various modes. Rolfs, and etc. [15] synthesized a new honeycomb lattice compound with more than 50% reduced sodium content by sodium removal from Na_2IrO_3 compound. The reduction of sodium content in the Na_2IrO_3 compound results in a change in symmetry from C2/c to P-3 in the iridium oxidation structure. Choi et al. [14] calculated and compared the measured frequencies and modes of Raman-active phonons at both ambient and high pressure with density functional theory (DFT) and dynamical mean field theory. Shitade et al. [15] studied the electronic states of Na_2IrO_3 compounds by first principle calculations. Malley et al. [10] examined the electronic band structure calculations of Li_2IrO_3 compounds using the Castep package program. They found that Li_2IrO_3 compound is metallic, Li_2PtO_3 compound is a semiconductor with 2.3 eV gap. Lüpke et al. [9] used the DFT, scanning tunneling microscopy and spectroscopy methods to predict the quantum spin Hall behavior of the Na_2IrO_3 compound. Chen et al. [16] calculated the electronic structure and average potential of Li_2IrO_3 compound using GGA and GGA + U approaches. Foyevtsova et al. [17] conducted a comprehensive analysis of the electronic properties of the Na_2IrO_3 compound by relativistic and non-relativistic DFT. Li et al. [18] investigated the electronic properties of γ - Li_2IrO_3 compound by the methods of relative DFT calculations and exact diagonalization of finite clusters and investigated the optical conductivity in detail.

As far as we know, it has not been determined that the theoretical studies on the mechanical properties and detailed spin polarized electronic band structure studies of $\text{X}_2(\text{X} = \text{Na}, \text{Li})\text{IrO}_2$ compounds have been performed. In this study, structural, mechanical, and electronic properties of $\text{X}_2(\text{X} = \text{Na}, \text{Li})\text{IrO}_2$ have been investigated.

2. Method of Calculation

In all of our calculations that were performed using the ab-initio total-energy and molecular-dynamics program VASP (Vienna ab-initio simulation program) [19–22] that

Table 1. The calculated equilibrium lattice parameters (a, b, and c) together with the experimental values and total magnetic moment (μ , in $\mu_B/\text{f.u.}$).

Material	Space group	a (Å)	b (Å)	c (Å)	V_0 (Å ³)	μ	Reference
Na ₂ IrO ₃	C2/m (No:12)	5.539	9.581	5.639	282.27	2.00	Bu çalışma ¹ Deney
		5.427	9.395	5.614	270.58		
Li ₂ IrO ₃	C2/m (No:12)	5.188	8.855	5.178	224.07	2.00	Bu çalışma ² Deney
		5.163	8.929	5.122	222.24		

was developed within the density functional theory (DFT) [23], the exchange-correlation energy function is treated within a spin polarized GGA (generalized gradient approximation) by the density functional of Perdew et al. [24]. The potentials used for the GGA calculations take into account the $1s^22s^1$ valence electrons of each Li-, $2p^63s^1$ valence electrons of each Na-, $2s^22p^4$ valence electrons of each O-, and $6s^24f^{14}5d^7$ valence electrons of each Ir- atoms. When including a plane-wave basis up to a kinetic-energy cutoff equal to 18.74 Ha for Na₂IrO₃ and 20.36 Ha for Li₂IrO₃, the properties investigated in this work are well converged. The Brillouin-zone integration was performed using special k points sampled within the Monkhorst-Pack scheme [25]. We found that a mesh of 5x5x4 k points and 5x5x5 k point for Na₂IrO₃ and Li₂IrO₃, respectively was required to describe the structural, mechanical, and electronic properties.

3. Result and Discussion

3.1. Structural Properties

As the first step in calculations, the lattice parameters of the Na₂IrO₃ and Li₂IrO₃ crystal structures have been calculated by optimization process. The optimized values of lattice parameters are given in Table 1. It is seen from Table 1 that the calculated lattice parameters are in agreement with the experimental results [4, 10]. The total magnetic moment value for both compounds has been calculated as 10 $\mu_B/\text{f.u.}$

3.2. Mechanical Properties

Here, the "strain-stress" method has been used to calculate elastic constants [26]. The 13 independent for monoclinic compounds elastic constants are calculated [27, 28]. The elastic constants calculated for Na₂IrO₃ and Li₂IrO₃ compounds are given in Table 2. Unfortunately, There are no theoretical and experimental results to be compare with the results here. The elastic constants calculated provide the mechanical stability conditions specified in the Ref. [28]. The polycrystalline Bulk modulus (B) and Shear modulus (G) are obtained from Voigt (V) -Reuss (R) -Hill (H) approximation [29–31] using the calculated elastic constants. The Young's modulus (E), Poisson ratio (ν), anisotropic factors, sound velocities and Debye temperature are also calculated from calculated Bulk module and Shear modules.

The bulk module gives a measure of the resistance shown against volume change, while the Shear modulus gives a measure of the resistance shown against shear stress. The Bulk (Shear) modules calculated for Na₂IrO₃ and Li₂IrO₃ are 143.8 (72.5) GPa and 181.7 (76.5) GPa, respectively. Young's modulus also gives a measure of stiffness.

Table 2. The calculated elastic constants (in GPa).

C_{ij}	Na_2IrO_3	Li_2IrO_3
C_{11}	265.9	290.3
C_{12}	99.7	144.2
C_{13}	97.9	136.5
C_{15}	-39.5	-40.8
C_{22}	256.7	269.7
C_{23}	101.4	139.5
C_{25}	40.7	45.3
C_{33}	189.0	242.5
C_{35}	1.1	7.6
C_{44}	84.5	60.6
C_{46}	41.3	45.9
C_{55}	90.1	129.5
C_{66}	90.6	129.8

Table 3. The calculated isotropic bulk modulus (B, in GPa), shear modulus (G, in GPa), Young's modulus (E, in GPa) and Poisson's ratio.

Material	B_R	B_V	B_H	G_R	G_V	G_H	E	ν	B/G
Na_2IrO_3	142.1	145.5	143.8	64.4	80.5	72.5	186.1	0.28	1.98
Li_2IrO_3	180.9	182.5	181.7	63.6	89.5	76.5	201.4	0.32	2.37

Table 4. The calculated anisotropic factors, sound velocities (v_t , v_l , v_m) and the Debye temperatures.

Material	A_B	A_G	A_1	A_2	A_3	$v_t(\text{m/s})$	$v_l(\text{m/s})$	$v_m(\text{m/s})$	θ_D (K)
Na_2IrO_3	1.20	11.15	1.31	1.48	1.12	3281	5976	3658	479
Li_2IrO_3	0.44	16.9	0.93	2.22	1.91	3187	6137	3567	504

If the Young's modulus is high, the material is stiffer. Young's values calculated for Na_2IrO_3 and Li_2IrO_3 are 186.1 GPa and 201.4, respectively. Therefore, we can say that these materials we examined are stiff materials. When B, G and E values are considered, it is seen that Li_2IrO_3 is a stiffer material than Na_2IrO_3 . The Poisson ratio value is 0.1 for covalent materials and 0.25 for ionic materials [32–34]. The calculated Poisson ratio values for Na_2IrO_3 and Li_2IrO_3 are 0.28 and 0.32, respectively. Therefore, the ionic contribution to internal atomic bonding for these compounds is dominant. A material is brittle (ductile) if its B/G ratio is less (higher) than 1.75 [35, 36]. These compounds are ductile as the B/G ratio for Na_2IrO_3 and Li_2IrO_3 is 1.98 and 2.37.

The elastic anisotropies (A_1 , A_3 , A_3) and the percentages of anisotropy (A_B , A_G) in the compression and shear, sound velocities and the Debye temperatures [37–39] calculated for Na_2IrO_3 and Li_2IrO_3 are given in Table 4. The Li_2IrO_3 compound exhibits high anisotropy compared to the Na_2IrO_3 compound. For materials, the A_B and A_G values can range from zero (isotropic) to 100% representing the maximum anisotropy [40]. The A_G calculated for the Li_2IrO_3 compound are higher than the Na_2IrO_3 compound. The Debye temperature value is high in hard materials and low in flexible materials. The Debye temperature value is large in hard materials and small in soft materials. The Debye temperature values of Na_2IrO_3 and Li_2IrO_3 compounds are 479 K and 504 K, respectively. Therefore, these compounds can be said to be hard materials. As in B, G and E, it is seen that Li_2IrO_3 compound is a harder material than Na_2IrO_3 compound.

Figure 1. The spin up and spin down electronic band structures for Na_2IrO_3 .

3.3. Electronic Properties

The electronic band structures of the Na_2IrO_3 and Li_2IrO_3 compounds have been calculated in k -space along the high symmetry points indicated in Figs. 1 and 2. The Fermi energy level has been pulled to zero energy. As seen in Fig. 1, the (-6-0) eV valence energy of band region is taken into account. The calculated E_g value for spin up and spin down of Na_2IrO_3 compound is 1.824 eV and 1.558 eV, respectively. In the spin polarized Na_2IrO_3 compound, the valence band maximum (VBM) for both spin up and spin down states is located at the A point and the conduction band minimum is located at the Z point. The calculated E_g value for spin up and spin down of Li_2IrO_3 compound is 2.315 eV and 2.019 eV, respectively. In the spin polarized Li_2IrO_3 compound, the VBM for both spin states is located at the Z point. These compounds exhibit wide band gap semiconductor behavior in both spin states.

The total and partial state densities corresponding to the electronic band structures of the Na_2IrO_3 and Li_2IrO_3 compounds are given in Fig. 3. The most natural description of the electronic structure of X_2IrO_3 is in terms of quasimolecular orbitals localized on a hexagon. The strongest Ir-Ir hopping is between 5d t_{2g} orbitals of neighboring iridium

Figure 2. The spin up and spin down electronic band structures for Li_2IrO_3 .

ions via common oxygens. In this case, an electron on a given Ir t_{2g} orbital propagates around an Ir_6 hexagon with the peculiarity that only a certain t_{2g} orbital at each Ir participates in the hopping. The t_{2g} degeneracy and bandwidth in Na_2IrO_3 are affected by structural distortions and the presence of Na in the Ir plane. This is revealed by calculations we have performed for a distortion- and Na-free hypothetical IrO_2 parent compound: while in IrO_2 the individual t_{2g} dispersions are as wide as 1.82 eV, the Na-induced band folding in Na_2IrO_3 opens large band gaps, leading to much narrower t_{2g} subbands [41–47]. Further, we have various possible hoppings between equal and different t_{2g} , as hoppings between unlike t_{2g} orbits via O 2p states and hoppings between unlike orbitals via O 2p and Na s states. In the Na_2IrO_3 , the energy region between –25 and –20 eV for both spin states is occupied by Na 2p states. The energy region between –20 and –15 eV for both spin states is occupied by O 2s states. The bands just below and above the Fermi energy level are occupied by Ir 4d and O 2p states. In the Li_2IrO_3 , the energy region between –45 and –40 eV for both spin states is occupied by Li s states. The energy region between –20 and –15 eV for both spin states is occupied by O 2s states. The bands just below and above the Fermi energy level are dominated by O 2p states. In the Li_2IrO_3 compound, the transitions from valence band to

Figure 3. The spin-polarized total and projected density of states for Na_2IrO_3 and Li_2IrO_3 compounds.

conduction band in both spin conditions are in p-d character while in the Na_2IrO_3 compound are s-p character.

4. Conclusion

In this work, the structural, electronic and mechanical properties of Na_2IrO_3 and Li_2IrO_3 have been calculated using the ab initio method. Spin polarized GGA approximation has been used in the calculations. The obtained lattice parameters values as a result of optimization are compared with the existing literature values, and it is seen that they are in agreement with these values. In electronic structure calculations, the X_2IrO_3 ($\text{X} = \text{Na}, \text{Li}$) compound for both spin up and spin down states are indirect wide gap semiconductor in nature. The calculated elastic constants provide the mechanical stability conditions. In addition, the calculated mechanical properties (bulk modulus, Shear modulus, Poisson's ratio, Young's modulus etc.) indicate that these compounds are ionic, rigid, and isotropic materials.

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References

1. D. Pesin and L. Balents, Mott physics and band topology in materials with strong spin-orbit interaction, *Nat. Phys.* **6** (5), 376 (2010). DOI: [10.1038/nphys1606](https://doi.org/10.1038/nphys1606).
2. J. Chaloupka, G. Jackeli, and G. Khaliullin, Kitaev-Heisenberg model on a honeycomb lattice: Possible exotic phases in iridium oxides $A_2\text{IrO}_3$, *Phys. Rev. Lett.* **105** (2), 027204 (2010). DOI: [10.1103/PhysRevLett.105.027204](https://doi.org/10.1103/PhysRevLett.105.027204).
3. H. Jiang *et al.*, Possible proximity of the Mott insulating iridate Na_2IrO_3 to a topological phase: Phase diagram of the Heisenberg-Kitaev model in a magnetic field, *Phys. Rev. B* **83** (24), 245104 (2011). DOI: [10.1103/PhysRevB.83.245104](https://doi.org/10.1103/PhysRevB.83.245104).
4. S. K. Choi *et al.*, Spin waves and revised crystal structure of honeycomb iridate Na_2IrO_3 , *Phys. Rev. Lett.* **108**, 127204 (2012).
5. J. Rodriguez, *Study of the Electronic Properties of Sodium Iridate*, (Riverside, University of California, 2019).
6. J. Kim *et al.*, Dynamic spin correlations in the honeycomb lattice Na_2IrO_3 measured by resonant inelastic x-ray scattering, *Phys. Rev. X* **10** (2), 021034 (2020). DOI: [10.1103/PhysRevX.10.021034](https://doi.org/10.1103/PhysRevX.10.021034).
7. H.-J. Kim, J.-H. Lee, and J.-H. Cho, Antiferromagnetic Slater insulator phase of Na_2IrO_3 , *Sci. Rep.* **4**, 5253 (2014). DOI: [10.1038/srep05253](https://doi.org/10.1038/srep05253).
8. Y. Singh, and P. Gegenwart, Antiferromagnetic Mott insulating state in single crystals of the honeycomb lattice material Na_2IrO_3 , *Phys. Rev. B* **82** (6), 064412 (2010). DOI: [10.1103/PhysRevB.82.064412](https://doi.org/10.1103/PhysRevB.82.064412).
9. F. Lupke *et al.*, Highly unconventional surface reconstruction of Na_2IrO_3 with persistent energy gap, *Phys. Rev. B* **91** (4), 041405 (2015). DOI: [10.1103/PhysRevB.91.041405](https://doi.org/10.1103/PhysRevB.91.041405).
10. M. J. O'Malley, H. Verweij, and P. M. Woodward, Structure and properties of ordered Li_2IrO_3 and Li_2PtO_3 , *J. Solid State Chem.* **181** (8), 1803 (2008). DOI: [10.1016/j.jssc.2008.04.005](https://doi.org/10.1016/j.jssc.2008.04.005).
11. F. Ye *et al.*, Direct evidence of a zigzag spin-chain structure in the honeycomb lattice: A neutron and x-ray diffraction investigation of single-crystal Na_2IrO_3 , *Phys. Rev. B* **85** (18), 180403 (2012). DOI: [10.1103/PhysRevB.85.180403](https://doi.org/10.1103/PhysRevB.85.180403).
12. A. Vasdev *et al.*, Dynamic surface modification due to effusion of Na in Na_2IrO_3 , *J. Appl. Phys.* **124** (5), 055102 (2018). DOI: [10.1063/1.5030606](https://doi.org/10.1063/1.5030606).
13. K. Rolfs *et al.*, Novel synthesis method of nonstoichiometric $\text{Na}_{2-x}\text{IrO}_3$ crystal structure, transport and magnetic properties, *J. Chem. Chem. Eng.* **10**, 153 (2016).
14. S. Choi *et al.*, Lattice dynamics and structural transition of the hyperhoneycomb iridate $\beta\text{-Li}_2\text{IrO}_3$ investigated by high-pressure Raman scattering, *Phys. Rev. B* **101**, 054102 (2020).
15. A. Shitade *et al.*, Quantum spin Hall effect in a transition metal oxide Na_2IrO_3 , *Phys. Rev. Lett.* **102**, 256403 (2009).
16. Y. Chen *et al.*, Electrical and lithium ion dynamics in Li_2IrO_3 from density functional theory study, *RSC Adv.* **4** (80), 42462 (2014). DOI: [10.1039/C4RA07793H](https://doi.org/10.1039/C4RA07793H).
17. K. Foyevtsova *et al.*, *Ab initio* analysis of the tight-binding parameters and magnetic interactions in Na_2IrO_3 , *Phys. Rev. B* **88**, 035107 (2013).
18. Y. Li *et al.*, Electronic excitations in $\gamma\text{-Li}_2\text{IrO}_3$, *Phys. Rev. B* **95**, 045129 (2017).
19. G. Kresse and J. Hafner, *Ab initio* molecular dynamics for liquid metals, *Phys. Rev. B* **47** (1), 558 (1993). DOI: [10.1103/physrevb.47.558](https://doi.org/10.1103/physrevb.47.558).
20. G. Kresse and J. Furthmüller, *Ab-initio* total energy calculations for metals and semiconductors using a plane-wave basis set, *Comput. Mater. Sci.* **6** (1), 15 (1996). DOI: [10.1016/0927-0256\(96\)00008-0](https://doi.org/10.1016/0927-0256(96)00008-0).

21. G. Kresse and D. Joubert D, From ultrasoft pseudopotentials to the projector augmented-wave method, *Phys. Rev. B.* **59** (3), 1758 (1999). DOI: [10.1103/PhysRevB.59.1758](https://doi.org/10.1103/PhysRevB.59.1758).
22. G. Kresse and J. Furthmüller, Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set, *Phys. Rev. B Condens. Matter Rev. B Matter.* **54** (16), 11169 (1996). DOI: [10.1103/physrevb.54.11169](https://doi.org/10.1103/physrevb.54.11169).
23. P. Hohenberg, and W. Kohn, Inhomogeneous electron gas, *Phys. Rev.* **136** (3B), B864 (1964). DOI: [10.1103/PhysRev.136.B864](https://doi.org/10.1103/PhysRev.136.B864).
24. J. P. Perdew, S. Burke, and M. Ernzerhof, Generalized gradient approximation made simple, *Phys. Rev. Lett.* **77** (18), 3865 (1996). DOI: [10.1103/PhysRevLett.77.3865](https://doi.org/10.1103/PhysRevLett.77.3865).
25. H. J. Monkhorst and J. D. Pack, Special points for Brillouin-zone integrations, *Phys. Rev. B.* **13** (12), 5188 (1976). DOI: [10.1103/PhysRevB.13.5188](https://doi.org/10.1103/PhysRevB.13.5188).
26. Y. L. Page and P. Saxe, Symmetry-general least-squares extraction of elastic coefficients from ab initio total energy, *Phys. Rev. B.* **63** (17), 174103 (2001). DOI: [10.1103/PhysRevB.63.174103](https://doi.org/10.1103/PhysRevB.63.174103).
27. J. P. Watt, Hashin-Shtrikman bounds on the effective elastic moduli of polycrystals with monoclinic symmetry, *J. Appl. Phys.* **51** (3), 1520 (1980). DOI: [10.1063/1.327803](https://doi.org/10.1063/1.327803).
28. Z.-J. Wu *et al.*, Crystal structures and elastic properties of superhard IrN₂ and IrN₃ from first principles, *Phys. Rev. B.* **76** (5), 054115 (2007). DOI: [10.1103/PhysRevB.76.054115](https://doi.org/10.1103/PhysRevB.76.054115).
29. W. Voight, *Lehrbook Der Kristallphysik* (Teubner, Leipzig, 1928); p. 962.
30. A. Reuss, Berechnung der fließgrenze von mischkristallen auf grund der plastizitätsbedingung für einkristalle, *Z. Angew. Math. Mech.* **9** (1), 49 (1929). DOI: [10.1002/zamm.19290090104](https://doi.org/10.1002/zamm.19290090104).
31. R. Hill, The elastic behavior of crystalline aggregate, *Proc. Phys. Soc. A.* **65** (5), 349 (1952). DOI: [10.1088/0370-1298/65/5/307](https://doi.org/10.1088/0370-1298/65/5/307).
32. V. V. Bannikov, I. R. Shein, and A. L. Ivanovskii, Electronic structure, chemical bonding and elastic properties of the first thorium-containing nitride perovskite TaThN₃, *Phys. Stat. Sol. (RRL)* **1** (3), 89 (2007). DOI: [10.1002/pssr.200600116](https://doi.org/10.1002/pssr.200600116).
33. H. Koc *et al.*, Ab initio calculation of the structural, elastic, electronic, and linear optical properties of ZrPtSi and TiPtSi ternary compounds, *Comput. Mater. Sci.* **62**, 235 (2012). DOI: [10.1016/j.commatsci.2012.05.052](https://doi.org/10.1016/j.commatsci.2012.05.052).
34. H. Koc *et al.*, First principles prediction of the elastic, electronic, and optical properties of Sb₂S₃ and Sb₂Se₃ compounds, *Solid State Sci.* **14** (8), 1211 (2012). DOI: [10.1016/j.solidstatesciences.2012.06.003](https://doi.org/10.1016/j.solidstatesciences.2012.06.003).
35. I. R. Shein and A. L. Ivanovskii, Elastic properties of mono- and polycrystalline hexagonal AlB₂-like diborides of s, p and d metals from first-principles calculations, *J. Phys: Condens. Matter.* **20** (41), 415218 (2008). DOI: [10.1088/0953-8984/20/41/415218](https://doi.org/10.1088/0953-8984/20/41/415218).
36. F. Pogh, Relations between the elastic moduli and the plastic properties of polycrystalline pure metals, *Philos. Mag.* **45**, 823 (1954).
37. I. Johnston *et al.*, *Solids State Physics Simulations, the Consortium for Upper Level Physics Software* (Wiley, New York, 1996).
38. O. L. Anderson, A simplified method for calculating the Debye temperature from elastic constants, *J. Phys. Chem. Solids* **24** (7), 909 (1963). DOI: [10.1016/0022-3697\(63\)90067-2](https://doi.org/10.1016/0022-3697(63)90067-2).
39. E. Schreiber, O. L. Anderson, and N. Soga, *Elastic Constants and Their Measurements* (McGraw-Hill, New York, 1973).
40. D. H. Chung and W. R. Buessem, in *Anisotropy in Single Crystal Refractory Compounds*, edited by FW Vahldiek, SA Mersol (Plenum, New York, 1968); p. 217.
41. S. Calder *et al.*, Enhanced spin-phonon-electronic coupling in a 5d oxide, *Nat. Commun.* **6**, 8916 (2015). DOI: [10.1038/ncomms9916](https://doi.org/10.1038/ncomms9916).
42. X. Liu *et al.*, Long-range magnetic ordering in Na₂IrO₃, *Phys. Rev. B.* **83** (22), 220403 (R) (2011). DOI: [10.1103/PhysRevB.83.220403](https://doi.org/10.1103/PhysRevB.83.220403).
43. P. Zheng *et al.*, Optical study on the possible Slater insulator SrIr_{0.8}Sn_{0.2}O₃, *Phys. Rev. B.* **100** (4), 045101 (2019). DOI: [10.1103/PhysRevB.100.045101](https://doi.org/10.1103/PhysRevB.100.045101).
44. R. Comin *et al.*, Na₂IrO₃ as a novel relativistic Mott insulator with a 340-meV gap, *Phys. Rev. Lett.* **109** (26), 266406 (2012). DOI: [10.1103/PhysRevLett.109.266406](https://doi.org/10.1103/PhysRevLett.109.266406).

45. Q. Cui *et al.*, Slater insulator in iridate perovskites with strong spin-orbit coupling, *Phys. Rev. Lett.* **117** (17), 176603 (2016). DOI: [10.1103/PhysRevLett.117.176603](https://doi.org/10.1103/PhysRevLett.117.176603).
46. T. Dziuba *et al.*, Surface conductivity of the honeycomb spin-orbit Mott insulator Na_2IrO_3 , *Phys. Status Solidi B.* **258** (1), 2000421 (2021). DOI: [10.1002/pssb.202000421](https://doi.org/10.1002/pssb.202000421).
47. Y. Zhang *et al.*, Strain-induced slater transition in polar metal LiOsO_3 , *Phys. Status Solidi RRL* **13** (12), 1900436 (2019). DOI: [10.1002/pssr.201900436](https://doi.org/10.1002/pssr.201900436).