Large bandgap and optical response of $d^0$ double perovskite $\text{Ba}_2\text{ScTaO}_6$

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(Dated: November 5, 2021)

Large bandgap insulators are considered promising for applications such as photocatalysts, dielectric resonators and interference filters. We investigate the electronic and optical properties of the synthesized $d^0$ double perovskite $\text{Ba}_2\text{ScTaO}_6$ which features unoccupied transition metal valence-$d$-states for Sc as well as Ta. Based on synchrotron X-ray diffraction and diffuse reflectance measurement, we report the crystal structure and the optical gap. Density functional theory based investigation of the electronic and optical properties within generalized gradient approximation shows a good qualitative agreement with the experimental findings, however the gap is severely underestimated. To reach a quantitative agreement, we consider different available flavours of the modified-Becke-Johnson exchange-correlation potential and discuss their effects on the electronic properties.

PACS numbers: 61.10.Nz, 78.20.-e, 71.15.Mb, 78.40.-q
Keywords: Double Perovskites, SXRD, UV-Vis spectroscopy, Kubelka-Munk, mBJ, DFT

I. INTRODUCTION

Double Perovskite oxides (DPOs), with the general formula $\text{A}_2\text{B'B'O}_6$, constitute an important materials class exhibiting a wide variety of interesting physical phenomena, like high temperature superconductivity, colossal magnetoresistance, photocatalytic activity, high dielectric constants, etc. [1–7]. In ordered systems, the transition-metals B and B’ are surrounded by oxygen atoms in an octahedral environment with B-O-B’ links. Therefore, DPOs consist of alternating corner sharing BO$_6$ and B’O$_6$ octahedra stacked in all three directions. On the other hand, the A-sites, centered at the interstitial voids created by these octahedra, are typically occupied by divalent alkaline earth metals or trivalent rare-earth metals. A schematic representation of ordered DPOs is shown in Fig. 1(b). The presence of different metal sites (A-, B- and B’-sites) allows a high degree of flexibility in crystal structure, opto-electronic and magnetic properties, responsible for the mentioned range of interesting phenomena. This further makes them appealing for novel device applications.

The large-gap $d^0$-DPOs formed by transition metals with unfilled/empty valence $d$-shells are of special interest [5–7]. They are considered promising in microwave-dielectric resonator applications, including interference filters, reflective coating and in optical fibres, due to their good dielectric properties, and as buffer materials due to their low reactivity. The properties of such materials are largely governed by the transition metal species and structural distortions [5, 6]. For example, it was found that the bandgap increases with increasing octahedral tilting and distortions. Moreover, difference in the electronegativity of the B and B’ cation can significantly affect the electronic bandgaps: compositional modulations can alter the bandgap by up to 2 eV. Therefore, to ascertain the feasibility of these materials for possible technological applications, a detailed characterization of their optical response over a wide frequency range is indispensable.

In this combined experimental and theoretical study, we focus on $\text{Ba}_2\text{ScTaO}_6$. Among the Ta-based DPOs, $\text{A}_2\text{MTaO}_6$, $\text{M} = \text{Sc}$ compounds are slightly different from other members of the family in terms of their bandgap [5]. Further, the electronic bandgap of $\text{Ba}_2\text{ScTaO}_6$ was predicted to be the smallest (3.35 eV) within the $\text{A}_2\text{ScTaO}_6$ compounds. With decreasing size of A cations, octahedral rotations and distortions induce a larger bandgap. The formal valency of Sc and Ta is, respectively, +3 and +5, leading to the $d^0$ configuration for both the involved transition metals. The ionic radii of the transition metal cations is found to be 0.745 Å and

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1 Ideally, DPOs have a cubic structure. However, depending on the size, A-site cations may induce tilt and rotations of the BO$_6$ and B’O$_6$ octahedra, leading to deviations from the ideal cubic structure. The resulting low-symmetry structure could be tetragonal, monoclinic, orthorhombic, or rhombohedral.
0.64 Å for Sc$^{3+}$ and Ta$^{5+}$, respectively. Large difference in the ionic radii is expected to lead to a long-range ordering of the BO$_6$ and BO$_8$ octahedra in the crystal structure. A good measure of the crystal structure symmetry is the tolerance factor [3–6]. For Ba$_2$ScTaO$_6$, the tolerance factor is found to be $t = 1.02$ [5], implying the likelihood of a cubic symmetry since $t \approx 1$.

The primary objective of this study was to ascertain the origin of low predicted bandgap of Ba$_2$ScTaO$_6$: whether this is an intrinsic property of the material or arises due to DFT approximations. To this end, we report the crystal structure, obtained via synchrotron X-ray diffraction (SXRD), and the optical gap, obtained via the diffuse reflectance measurement in the UV-Vis range. We find that Ba$_2$ScTaO$_6$ crystallizes in an ordered cubic structure and has a gap of $\sim 4.5$ eV, similar to other A$_2$MTaO$_6$ (M = Y, Al and Ga). For the synthesized DPO Ba$_2$ScTaO$_6$, we have performed a thorough investigation of the electronic and optical properties within the framework of density functional theory (DFT). Standard DFT using generalized gradient approximation (GGA) agrees with the earlier reports. A quantitative agreement between theory and experiments is, however, found only upon including the modified Becke-Johnson (mBJ) exchange-correlation potential. This leads to accurate predictions for the optical response. Inclusion of the mBJ potential reduces the conduction bandwidth of the $t_{2g}$ states and increases the bandgap. In particular, our comparative study of different different parametrizations of the mBJ potential clarifies the most suitable choice of mBJ potential for Ba$_2$ScTaO$_6$ and likely also for other materials with similar bandgap and electronic properties.

II. EXPERIMENTAL AND COMPUTATIONAL DETAILS

A. Synthesis, characterization and optical gap

Off-white samples of Ba$_2$ScTaO$_6$ were synthesized using the solid-state reactions at 1500 °C for 72 hours. Synchrotron X-ray Diffraction (SXRD) study were carried using BL-11 of Indus-2 synchrotron source [8], using $\lambda = 0.46195$ Å beam with a beam current of 100 meV and energy 2.5 GeV, at the Raja Ramanna Center for Advanced Technology (RRCAT), Indore, India. The Rietveld analysis software FULLPROF [9] was used to analyze the SXRD data, which shows a cubic structure, space group $Fm\bar{3}m$ (No. 225). Ba, Sc, Ta, and O atoms occupy the the Wyckoff positions of 8c, 4a, 4b and 24e, respectively. The SXRD pattern and the Rietveld fit is shown in Fig. 1(a). The crystal structure is shown in Fig. 1(b) and the corresponding details related to the structural and the refinement parameters are listed in Table I. Diffusive reflectance spectroscopy were carried out in the UV-Vis frequency range using the UV-Vis-NIR spectrophotometer Perkin-Elmer 950. The reflectance spectra was converted into the Kubelka-Munk (KM) function, $F(R) [10, 11]$. The optical bandgap was calculated using [6]:

$$F(R) \propto \frac{(h\nu - E_g)^n}{h\nu},$$

with $n = 1/2$ corresponds to direct-allowed transitions. $h\nu$ and $E_g$ are the incident photon energy and the gap, respectively. As outlined in [6], the intercept of the linear part of $[F(R)h\nu]^2$ vs $h\nu$ curve on the energy axis is the bandgap. Figure 1(d) shows the absorption spectra and the corresponding value of bandgap. The value of the bandgap was found to be 4.57 eV.

B. Density functional theory

We adopted the all electron full-potential linearized augmented plane wave (FP-LAPW) method of DFT with the scalar relativistic approximation, as implemented in the WIEN2k code [12, 13]. All calculations were carried out for the experimental crystal structure (Table I), using a $12 \times 12 \times 12$ $k$-mesh in the full Brillouin zone (BZ) ($\sim 72$ $k$-points in the irreducible Brillouin zone) to carry out the integrals over the BZ. The muffin-tin radii for Ba, Sc, Ta, and O were kept fixed at 2.5 a.u., 2.3 a.u., 2.03 a.u. and
with the earlier reported X-ray diffraction data in the
respectively. These values are in excellent agreement
Symmetry the Sc-O-Ta angle is 180°. Within the cubic
Crystal structural are listed in Table I. For a cubic structure, for example, the
dent components. However, depending on the crystalline
related by Kramers-Kronig relation:
ε(ω) = ε1(ω) + iε2(ω).
In general, ε is a second rank tensor with nine indepen-
dent components. However, depending on the crystalline
symmetry, only a few of these components could be
independent. For a cubic structure, for example, the
three principle directions (x, y, and z) are equivalent,
leading to only one independent value. The real and
imaginary part of the electric response function are
related by Kramers-Kronig relation:
ε1,ij(ω) = δij + \frac{2}{\pi} P \int_0^\infty \frac{\omega' \varepsilon_{2,ij}(\omega')}{\omega'^2 - \omega^2} d\omega' (3)
where P stands for the principal part of the integral
and εa,ij is the ij-th component of εa (a = 1, 2). All
other optical response functions, such as the refractive
index, optical conductivity, absorption coefficient and
the electron loss function, were obtained by using their
well-defined mathematical relations with the dielectric
function [18]. The broadening parameter was chosen to
be 0.1 eV.

III. RESULTS AND DISCUSSIONS

A. Crystal structure and optical bandgap

Ba2ScTaO6 crystallizes in a cubic Fm\overline{3}m structure (No. 225) with lattice constant a = 8.226 Å. The only free
parameter in this structural model, viz. the x-coordinate
for the O atom is found to be x = 0.245 based on a
high-resolution SXRD data. The complete details of the
crystal structural are listed in Table I. Within the cubic
symmetry the Sc-O-Ta angle is 180°. The M-O bond
lengths are 2.0894 Å and 2.0236 Å, for M=Sc and Ta,
respectively. These values are in excellent agreement
with the earlier reported X-ray diffraction data in the
Springer Materials database [19, 20], but deviate slightly
from the prediction based on SPuDS [21].

TABLE I: Crystal structure and refinement parameters

| Atoms | WP | x     | y     | z     | B (Å) |
|-------|-----|-------|-------|-------|-------|
| Ba    | 8c  | 1/4   | 1/4   | 1/4   | 0.12(2) |
| Sc    | 4b  | 1/2   | 1/2   | 1/2   | 0.11(1) |
| Ta    | 4a  | 0     | 0     | 0     | 0.23(1) |
| O     | 24c | 0.245(3) | 0    | 0     | 0.08(0) |

Figure 1(d) shows the modified KM function (see Sec. II A), corresponding to direct optical bandgaps, as a
function of the incident photon energy. The bandgap is
obtained by taking the intercept of the low-energy linear
part of this curve on the energy axis [6, 10, 11]. The
bandgap is found to be 4.57 eV, which is consistent with
the off-white color of the sample.

B. Electronic properties

DFT calculation using GGA leads to a non-magnetic
insulating ground state for Ba2ScTaO6. The correspond-
ting total and partial densities of states (DOS) are shown
in Figure 2(a), clearly exhibiting the insulating nature.
The electronic properties of insulator DPOs can be well-
described by the crystal field experienced by the M-d
states and hybridization between the oxygen 2p states
and the M-d states. The crystalline field produced by
the nearest oxygen atoms in an octahedral geometry
lifts the five-fold degeneracy of M-d states and leads
to splitting into the lower lying t2g states, consisting of
dxy, dxz, and dyz orbitals, and eg states, consisting of
dz2-y2 and dx2-z2 orbitals. Typical of DPOs, hybridization
with the surrounding oxygen atoms leads to bonding states
with dominant contribution from the O-p orbitals in
valence band while the conduction band edge comprises
of anti-bonding states with dominant d contribution. The
relative energy position of the transition metal d states,
however, depends on the metal species (electronegativity,
formally unoccupied (d⁰-ness), the M-d states (both t₂g and e₂g states) for M=Sc as well as M=Ta lie in the conduction band, as shown in Fig. 2(a). This, in turn, confirms the formal valency of +3 and +5 for Sc and Ta, respectively.

As observed from the atom- and orbital-resolved density of states (DOS), the conduction band edge states have dominant contribution from the Ta-t₂g states with small contributions from Sc-t₂g states. This is somewhat different from A₂YTaO₆ DPOs [5] despite similar electronegativity of Y (1.22) and Sc (1.36) (1.61). In comparison, the electronegativity of Ta is 1.50. The primary reason for this difference is the relatively small energetic overlap between the Y-4d and O-2p states as compared to Sc-3d and O-2p states. Strong covalency effects between Sc-O and Ta-O are also noted. The dominant Ta-t₂g and Ta-e₂g contribution is found at ~ 4.5 eV and ~ 10 eV, respectively, implying a crystal field splitting of approximately 5.5 eV. On the other hand, the crystal field splitting for Sc-d states is merely ~ 2.2 eV, a consequence of relative electronegativity difference and M-O distances. The relative hybridization between Sc-O is found to be quite smaller that Ta-O as evidenced by the M-d DOS in the valence band region. Therefore, an appropriate description of the electronic structure is (large) mixing of Sc-3d states with the strongly hybridized Ta-O anti-bonding states.

As shown in Fig. 2(b), the electronic bandstructure within GGA has a direct gap of ~ 3.1 eV, which is much smaller than the gap estimated from the UV-Vis reflectance spectroscopy. This discrepancy between the theoretical and experimental estimates is a well-known issue within DFT. A computationally efficient way to address this discrepancy is to employ the Tran-Blaha modified-Becke-Johnson (TB-mBJ) exchange-correlation potential [15].

Inclusion of such correction leads to a remarkable improvement in the comparison between the measured and the calculated electronic gap, as shown in Fig. 3(a) & (b). The electronic bandgap within TB-mBJ is approximately 4.25 eV, much closer to the experimental value (only ~ 7% smaller). Other aspects of the electronic properties only undergo quantitative changes. The conduction band edge has relatively large contribution from Sc-d orbitals, implying further enhancement of covalency effects. This is accompanied by reduction of the effective crystal field splitting for the Sc-d state to ~ 1 eV. For Ta-d states in comparison, the crystal field splitting undergoes only marginal change. The bandwidth of the d states, for both Sc and Ta, is slightly reduced. It is important to note that these corrections are not a rigid shift of all the conduction band states (“scissors” operation), and, therefore, may significantly influence the optical properties. In comparison to GGA, a simplified view of the application of the orbital-dependent corrections introduced by the mBJ potential could be a band-dependent scissors operation like shifts [22].

Despite its successes, TB-mBJ potential is known to underestimate the gap in many cases [16]. Different parametrizations of the mBJ potential have, therefore, been suggested which are specifically catered to perovskite oxides [16], halide perovskites [17], and large bandgap materials [16]. To further improve the degree of comparison between calculated and measured gap, we first tried the mBJ potential adapted for perovskite oxides (labelled mBJ-1). The resulting bandgap is found to be approximately 4.36 eV. While the situation is improved as compared to TB-mBJ, surprisingly it is still ~ 4.5% smaller. On the other hand, the version adapted for perovskite halides (labelled mBJ-3), leads to an overestimation presumably due to large electronegativity difference between ligand species (oxygen vs halides). The resulting bandgap is found to be ~ 5.5 eV. An excellent agreement is, however, found for the mBJ potential adapted for large bandgap insulators (labelled mBJ-2). These results are summarized in Table II for brevity, with details related to their implementation in WIEN2k.

The bandgap within mBJ-2 is found to be 4.61 eV which is almost identical to the experimental estimate of 4.57 eV. In terms of the electronic properties, as shown in Fig. 3(c) and (d), DOS and bandstructures are qualitatively similar to TB-mBJ and shows only small quantitative changes. In view of this excellent agreement, to study the optical properties, we consider only the mBJ-2 case.

C. Optical properties

Finite-frequency optical response of materials is captured through their complex dielectric function ε_{μν}(ω) (μ, ν = x, y, z). For structures with cubic symmetry, only one component of ε_{μν} is independent as ε_{xx} = ε_{yy} = ε_{zz}. The symmetry relation between different components also holds for other optical response functions.

The dielectric function for Ba₂ScTaO₆ for the mBJ-2 method is shown in Fig. 4(a)-(b). The onset of the optical response ε₂ is at a finite frequency, at ~ 4.5 eV, due to the finite electronic bandgap. The peaks in ε₂(ω) correspond to optical transitions from states in the valence band to states in the conduction band and is proportional to the joint DOS between the initial and final states involved in such transitions. In general, the optical selection rules dictate if such transitions are allowed. In the present case, as also for most insulating DPOs, the valence band and conduction band states close to the Fermi energy are dominantly of O-2p and M-d characters. As a result, the selection rules are trivially satisfied. Indeed, the transitions between the O-2p states in the valence band and M-d states at the conduction band edge lead to the optical transitions in the entire energy range studied. For example, the features below ~ 6.5 eV can be understood as transitions from the
valence band region to the conduction band edge (Ta-$t_{2g}$ states). Similarly, prominent peak in $\varepsilon_2$ at $\sim 7$ eV and $\sim 11.5$ eV arise due to transitions from valence band edge to the Sc-$t_{2g}$ states and transitions from valence band edge to Ta-$e_g$ states, respectively.

The frequency-dependence of the real and imaginary parts of the refractive index closely follow the complex dielectric function, as shown in Fig. 4(c)-(d). They, respectively, correspond to the dispersion and absorption of light passing through the medium. The refraction coefficient peaks at the photon energy of 5.5 eV approximately and reaches a maximum value of $\sim 2.4$. The static refractive index, $n(\omega = 0)$, is obtained from the static limit of the real part of the dielectric function: $n = \sqrt{\varepsilon_1(\omega \rightarrow 0)}$, and is found to be 1.72.

The complex optical conductivity $\sigma(\omega) = i\omega\varepsilon(\omega)/4\pi$ is
Table II: Electronic bandgap obtained within different DFT approximations.

| Method       | Gap (eV) | Remarks                                      |
|--------------|----------|----------------------------------------------|
| Experimental | 4.57     | UV-Vis spectroscopy                          |
| PBE-GGA      | 3.12     |                                              |
| TB-mBJ       | 4.25     | “Option 0” in WIEN2k, defined in Ref. [15].  |
| mBJ-1        | 4.36     | modified mBJ parameters suitable for perovskite oxides; |
|              |          | “Option 1” in WIEN2k, defined in Ref. [16].   |
| mBJ-2        | 4.61     | modified mBJ parameters suitable for large bandgap materials; |
|              |          | “Option 2” in WIEN2k, defined in Ref. [16].   |
| mBJ-3        | 5.48     | modified mBJ parameters suitable for halide perovskites |
|              |          | “Option 4” in WIEN2k, defined in Ref. [17].   |

Fig. 4: The (a) real $\varepsilon_1(\omega)$ and the (b) imaginary $\varepsilon_2(\omega)$ parts of the dielectric function. The (c) real $n(\omega)$ and the (d) imaginary $k(\omega)$ parts of the refractive index.

shown in Fig. 5(a)-(b). The low-energy peaks in the real part of the optical conductivity exhibit characteristics similar to the dielectric function $\varepsilon_2(\omega)$, with the prominent peaks at $\sim 7$ eV, $\sim 9.3$ eV, $\sim 10$ eV and $\sim 11.5$ eV. The dispersive part of the dielectric function, $\varepsilon_1(\omega)$, governs the imaginary part of the optical conductivity. It is negative for small values of photon energy and crosses zero around 10 eV. The zero-crossing energy is consistent with the that of $\varepsilon_1(\omega)$, as expected.

As shown in Fig. 5(c), the absorption edge lies at $\sim 4.5$ eV and increases with increasing photon energy. The finite value of the absorption edge is due to the bandgap. The peaks around the energies 7 eV and above arise due to inter-band transitions, as discussed earlier.

The Loss function, $L(\omega)$, corresponds to the electron energy loss spectroscopy (EELS) which captures both non-scattering and elastic scattering processes. It is connected to the energy loss of the electrons as they traverse through the medium and loose energy. Typically, the mixing of single electron excitations with the collective excitations (plasmons) gives rise to energy loss of the electrons up to 50 eV.

The loss function for Ba$_2$ScTaO$_6$ and is shown in Fig. 5(d) and qualitatively follows the imaginary part of the dielectric function $\varepsilon_2(\omega)$. There are two prominent peaks, lying at $\sim 7$ eV and $\sim 10.6$ eV. The first (low-energy) peak at $\sim 7$ eV, originate from inter-band transitions between O-2$p$ to M-–d states as discussed earlier, while the latter originates from transitions between semi-core states to conduction band edge.

IV. CONCLUSIONS

To summarize, we have experimentally determined the crystal structure and optical bandgap of Ba$_2$ScTaO$_6$ and theoretically investigated its electronic and optical properties. Contrary to the earlier prediction based on
GGA, the experimental gap of Ba$_2$ScTaO$_6$ is found to be $\sim 4.6$ eV, which is similar to other Ta-based $d^0$-DPOs. An excellent quantitative agreement between experiment and DFT is obtained upon considering also the adapted mBJ potential suggested for large gap insulators. Other mBJ potential considered in this study, although better than GGA, still performs rather poorly, including the one adapted for perovskite oxides.

Due to its large bandgap, Ba$_2$ScTaO$_6$ is a potential functional material and may find use as microwave dielectric resonators, interference filters, buffer materials as well as in photocatalysis. Detailed and accurate optical properties have been obtained with mBJ-2. Our comparative analysis of different mBJ flavours will also prove useful for other similar DPOs.

**Acknowledgements**

AKH and SK thank Dr. V. Srihari for the SXRD experimental support at BL-11, RRCAT, Indore. RR thanks Ulrike Nitzsche for technical assistance with the computational resources in IFW Dresden.

**Competing Interests**

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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