Evaluation of the electron-TO-phonon interaction
in polar crystals from experimental data

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The aim of this study was to determine the strengths of the coupling of electrons with the polar long-wavelength transverse optical (TO) vibrations from infrared spectroscopy data. This determination is made by means of a simple relationship between the electron-TO-phonon interaction constant and material parameters, based on a parametrization of the electron-TO-phonon coupling in terms of the long-range dipole-dipole interaction. The combination of experimental data employed here allowed us to calculate directly the relevant constants for a number of representative polar insulators and to show that in ferroelectrics the interband electron-TO-phonon interaction at the Γ point is essentially strong. In these calculations, infrared spectroscopy methods proved to be an effective tool for study of the main properties of electron interaction with polar long-wavelength TO phonons.

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I. INTRODUCTION

In solid state science, there are a number of techniques for probing detailed characteristics related to the structural and dynamical properties of materials, which are therefore capable of numerical prediction of electron-phonon coupling constants from experimental data. In particular, methods of vibrational spectroscopy have been shown to yield reliable estimates of several fundamental microscopic parameters, including relevant constants of electron-phonon interactions (e.g., [1–5] and references therein).

Two common properties of the lattice dynamics of a polar crystal are (i) the existence of dipole moments associated with optical vibrational modes and (ii) the difference in long-range fields given by longitudinal and transverse optical modes at the zone center [6]. As shown in our previous study [7], in polar materials, the coupling of electrons with the polar long-wavelength transverse optical (TO) vibrations is essentially influenced by the features of the Coulomb interaction between electrons and the lattice ions. In turn, these features are directly related to the presence of the dipole moments of the TO vibrational modes. At the same time, dependencies of the dipole moments on the ionic degrees of freedom give rise to infrared (IR) spectra [8, 9], which makes IR spectroscopy an important tool for investigating the low-frequency dynamics of the IR-active TO modes in polar materials (e.g., [10]).

The characteristics of the IR spectra can be understood in terms of effective charges belonging to the TO vibrational modes. The relative values of these charges are directly related to the strength of the corresponding long-range electron-TO-phonon couplings [2]. By combining these features, we see that information on the intensities of IR-active vibrations provided by IR spectroscopy measurements can be successfully used for quantitative modeling of the interactions of electrons with zone-center TO phonon modes. Thus, the analysis of the IR spectra data in terms of the dielectric function can serve as an alternative to ab-initio methods to obtain from an experiment independent estimates of the electron-TO-phonon (el-TO-ph) coupling constants in a given material.

To the best of our knowledge, with only a few exceptions, no direct estimates of the el-TO-ph interaction constants were previously available to provide numerical values for most polar materials, especially for ferroelectric systems in which the strength of the el-TO-ph interaction should be especially strong [7]. In particular, even for several well-studied compounds, such as BaTiO₃, SrTiO₃, and SnTe, there was little information on how different or similar the relevant constants of the electron-TO phonon coupling are. In this work, we have performed a numerical investigation of the el-TO-ph interaction constants for a number of representative polar compounds using the theoretical scheme proposed in [7]. To obtain a more detailed picture, we present a comparative analysis of the results of our calculations. As expected [7], very large values of the interband el-TO-ph interaction constants were found to be a general feature of ferroelectric materials.
II. THEORETICAL DETAILS

Contributions of the IR active optical phonons to the dielectric function $\epsilon(\omega)$ of the far-IR spectral range, which are the subject of IR spectroscopy measurements and analysis, are usually modeled by a classical damped harmonic oscillator model \[10, 11]:

$$
\epsilon(\omega) = \epsilon_\infty + \sum_j \frac{S(j)}{\Omega_j^2 - \omega^2 - i\gamma_j \omega}
$$

with $\Omega_j$, $\gamma_j$ and $S(j)$ the $j$-th zone-centre TO vibrational mode frequency, damping and dipole oscillator strength, respectively; $\epsilon_\infty$ is the core (electronic high-frequency) contribution to the dielectric function.

In our previous work \[7\], within a first-principles methodology, we predicted theoretically the significant increase of the constants of the el-TO-ph coupling in ferroelectric materials, showed how the el-TO-ph interaction constants might be dependent on macroscopic material parameters, and obtained analytical equations allowing us to estimate el-TO-ph interaction strengths in a wide range of polar dielectrics. In the limit of a zero phonon wave-vector, the el-TO-ph interaction represents the long-range electron-lattice dynamic hybridization of the electronic bands of opposite parities, which takes into account the relevant

\[\text{Contribution of the IR active optical phonons to the dielectric function behavior in the far-IR spectral range, and using Eqs. (3) in combination with the experimental data for } \epsilon_\infty \text{ and } E_\sigma, \text{ enables us to determine numerical values of the el-TO-ph coupling constants for polar systems of interest.}\]
TABLE I: The calculated values of the el-TO-ph interaction constants provided for each polar TO mode of a cubic phase of the ferroelectric ABO$_3$ perovskite oxides and A$^{IV}$/B$^{VI}$ narrow-gap semiconductors. The material parameters used are also given.

| Compound    | $\epsilon_\infty$ | $E_g$ | $M_j S(j)$ | g$_{0j}$ | g$_j$ | $\kappa_j$ | $K_0$ |
|-------------|--------------------|-------|------------|---------|-------|-----------|-------|
|             | (eV)               | (eV)  | (eV/$\AA^2$) | (eV/$\AA$) | (eV/$\AA$) | (eV/$\AA^2$) | (eV/$\AA^2$) |
| BaTiO$_3$   | 5.2                | 3.3   | 1          | 194.3   | [32]  | 7.3       | 4.7   | 2.41 | 2.80 |
|             | [30] [31]          | 2     | 15.1      | 2       | 1.3   |           |       |      |      |
|             | [30] [31]          | 3     | 7.8       | 1.5     | 0.9   |           |       |      |      |
| SrTiO$_3$   | 5.2                | 3.3   | 1          | 211.6   | [32]  | 7.6       | 4.9   | 2.42 | 3.04 |
|             | [30] [33] [34]     | 2     | 18.8      | 2.3     | 1.5   |           |       |      |      |
|             | [30] [33] [34]     | 3     | 18.1      | 2.2     | 1.4   |           |       |      |      |
| KNbO$_3$    | 4.7                | 3.1   | 1          | 246.4   | [36]  | 8.0       | 5.3   | 3.27 | 2.81 |
|             | [30] [35]          | 2     | 24.3      | 2.5     | 1.7   |           |       |      |      |
|             | [30] [35]          | 3     | 33.0      | 2.9     | 2.0   |           |       |      |      |
| KTaO$_3$    | 4.6$^a$            | 3.6   | 1          | 211.0   | [38]  | 8.0       | 5.4   | 2.81 | 2.85 |
|             | [37]               | 2     | 24.3      | 2.7     | 1.8   |           |       |      |      |
|             | [37]               | 3     | 28.4      | 2.9     | 2.0   |           |       |      |      |

$^a$ estimated as in Ref. [30]

III. RESULTS AND DISCUSSION

We performed numerical calculations with Eqs. [3] for representative polar compounds belonging to several classes of materials: typical insulating perovskites, the A$^{IV}$/B$^{VI}$ narrow-gap semiconductors, and various non-ferroelectric wide-gap binary compounds. The evaluation of $g_{0j}$ and $g_j$ for these compounds involved the knowledge of material parameters ($S(j)$, $\epsilon_\infty$, $E_g$) whose experimental values were taken from the literature or, when necessary, calculated from the corresponding experimental data. Lists of all compounds considered and the calculated el-TO-ph coupling constants and material parameters used are given in Tables 1 and 2.

Additionally, in both tables we presented the values of the dimensionless coupling parameter $\kappa_j = g_j^2/(E_g K_0)$ calculated for low-frequency TO modes. Here $K_0 = 4\pi\epsilon/\nu_0$, and $\nu_0$ is the cell volume with respect to the formula unit. From a physical point of view, $\kappa_j$ is represented as a ratio of the electronic contribution $g_j^2/E_g$, determined by the electronic structure and the electron-ion potential, and some lattice force constant $K_0$. This specially introduced parameter is of considerable interest due to its direct ability to supply a measure of the zone-center TO phonon softening arising from the interband scatterings of the bond electrons. As seen from Tables 1 and 2, only the wide-gap ferroelectric materials are characterized by the high values of the parameter $\kappa$. Since in the cubic binary crystal systems one can set $j = 1$, we also omitted the indices $j$ throughout Table 2. Note that for the most part of binary compounds represented in this table, we calculated the dipole oscillator strengths $S$ with the following correspondence: $(\Omega_{LO}^2 - \Omega_{TO}^2) \epsilon_\infty = S$ which relates the squared frequencies of the longitudinal and transverse zone-center optical vibrations, $\Omega_{LO}$ and $\Omega_{TO}$, respectively, with $S$.

Based on the comparative analysis of the results obtained and summarized in both tables, we can draw several general conclusions and discuss the role of the el-TO-ph coupling related to the ferroelectricity phenomenon:

i) A simple calculation recently proposed in [7] as a quantitative measure of the el-TO-ph interaction is shown to be applicable for a wide number of selected polar insulators and semiconductors, including representative ferroelectric compounds.

ii) Among the compounds considered, it was clearly demonstrated that the el-TO-ph coupling strength is small in alkali halides, intermediate in binary oxides, both the alkaline earth and 3d-transition metals, and, in contrast to the first two cases, significantly large in ferroelectric perovskites. Notice also that the values of the el-TO-ph coupling constants $g_j$ tabulated in Table 1 for A$^{IV}$/B$^{VI}$ compounds agree with the relevant values from semi-empirical estimates [12]. The values of $g_j$ given in Table 1 for the wide-gap ferroelectrics can be compared with the only known semi-empirical estimate of Ref. [12] for BaTiO$_3$, which, in turn, should be recast by applying the accurate magnitude of the effective
TABLE II: The calculated values of the el-TO-ph interaction constants in a number of cubic binary crystal systems. The material parameters used are also given.

| Compound                  | $\epsilon_\infty$ | $E_g$  | $MS$  | Ref. | $g_0$  | $g$  | $\kappa$ | $K_0$  |
|---------------------------|-------------------|--------|-------|------|--------|------|---------|--------|
|                           | (eV)              | (eV/Å²)| (eV)  |       | (eV/Å) | (eV/Å) | (eV/Å²) |
| **Oxides of the alkaline earth metals** |                   |        |       |      |        |      |         |        |
| MgO                       | 2.95              | 7.2    | 36.2  | [42, 43] | 4.7   | 3.6  | 0.19    | 9.67   |
| CaO                       | 3.38              | 6.2    | 33.6  | [43, 44] | 4.2   | 3.1  | 0.24    | 6.50   |
| SrO                       | 3.28              | 5.3    | 29.4  | [43, 44] | 3.6   | 2.7  | 0.26    | 5.26   |
| BaO                       | 3.61              | 4.0    | 31.0  | [43, 44] | 3.2   | 2.4  | 0.33    | 4.26   |
| **Transition-metal magnetic monoxides** |                   |        |       |      |        |      |         |        |
| MnO                       | 4.85              | 3.6    | 52.8  | [45, 46] | 4.0   | 2.6  | 0.23    | 8.24   |
| NiO                       | 5.61              | 3.7    | 45.5  | [44, 46] | 3.7   | 2.4  | 0.15    | 9.93   |
| CoO                       | 5.00              | 2.8    | 45.1  | [46, 47] | 3.2   | 2.1  | 0.17    | 9.36   |
| FeO                       | 5.38              | 2.4    | 43.5  | [44, 46] | 2.9   | 1.9  | 0.16    | 9.05   |
| **Alkali halides**        |                   |        |       |      |        |      |         |        |
| LiCl                      | 2.70              | 9.4    | 7.0   | [48, 49] | 2.3   | 1.9  | 0.07    | 5.33   |
| NaCl                      | 2.33              | 8.5    | 4.9   | [40, 48] | 1.9   | 1.6  | 0.07    | 4.03   |
| KCl                       | 2.20              | 8.4    | 3.7   | [43, 48] | 1.6   | 1.4  | 0.08    | 2.90   |
| RbCl                      | 2.20              | 8.2    | 3.5   | [43, 48] | 1.5   | 1.3  | 0.08    | 2.54   |
| LiF                       | 1.90              | 13.7   | 11.0  | [43, 49] | 3.5   | 3.1  | 0.06    | 11.08  |
| NaF                       | 1.74              | 11.5   | 7.5   | [43, 49] | 2.7   | 2.4  | 0.07    | 7.24   |
|KF                         | 1.85              | 10.8   | 5.9   | [43, 49] | 2.3   | 2.0  | 0.08    | 4.73   |
| **Thallium and cesium halides** |                   |        |       |      |        |      |         |        |
| TlCl                      | 4.76              | 3.2    | 13.7  | [50]  | 1.9   | 1.3  | 0.16    | 3.21   |
| TlBr                       | 5.34             | 2.65   | 12.6  | [51]  | 1.7   | 1.1  | 0.15    | 2.89   |
| CsCl                      | 2.63              | 8.3    | 4.4   | [40, 48] | 1.7   | 1.4  | 0.09    | 2.58   |

charge: using the value 8.33 estimated from the data of Table 1, one obtains the corrected estimate 4.2 eV/Å, which is close to the value 4.7 eV/Å of Table 1 for BaTiO₃.

iii) There is a nontrivial one-to-one correspondence with the zone-center TO vibrational mode effective charge $Z^*$, or equally with the Born effective charge. It is seen that the charge $Z^*$ sets the scale of the el-TO-ph coupling; for instance, in pure ionic wide-gap materials, where the Born effective charges are very close to the nominal rigid-ion values, the actual el-TO-ph coupling strength is small. To further quantify the interplay between these physical quantities, we plot their interrelation in Fig. 1, which uniquely displays the substantial growth of the el-TO-ph coupling with a rise in the effective charge: $\kappa \propto |Z^*|^2$, just as predicted \cite{7}. Due to the anomalously large Born effective charges, which occur in ferroelectric compounds \cite{30, 52}, a marked increase in interband hybridization leads to a drastic enhancement of the interband el-TO-ph scatterings. In the limit of pure ionic wide-gap compounds, multiband channels of electronic scatterings associated with zone-center TO phonons turn out to be marginal, as the electronic polarizability effects are not high enough to exhibit a noticeable el-TO-ph hybridization between different bands. Thus, our calculations show that strong el-TO-ph coupling should be a general feature of wide-gap compounds with high electronic polarizabilities.

As a matter of fact, the same results hold in the case of $A^IVB^VI$ narrow-gap semiconductor systems where, however, one should take into account two factors: smallness of $E_g$ and sufficiently high range of $\epsilon_\infty$. It is easy to see from Table 1 that the relevant values of the product $M_jS(j)$ for both wide-gap and narrow-gap ferroelectrics appears to be close to each other. At the same time, in non-ferroelectrics, as seen from Table 2, these values are significantly smaller. Moreover, for both groups of ferroelectrics, the unscreened dimensionless el-TO-ph coupling parameter, $\kappa_0(\epsilon_\infty + 2)/3$, as seen from Table 3, turns out to be about the same order of magnitude. Meanwhile, for the non-ferroelectric compounds considered, the values of this parameter differ significantly and are much smaller than in the ferroelectrics.
TABLE III: The calculated values of the unscreened dimensionless $\text{el-TO-ph}$ coupling parameter for a selected number of polar compounds in a cubic phase.

| Compound | $\kappa_j (\epsilon_\infty + 2)^{-1/2}$ |
|----------|------------------|
| KNbO$_3$ | 7.3              |
| BaTiO$_3$| 5.8              |
| PbTe     | 5.8              |
| SnTe     | 4.3              |
| PbSe     | 2.4              |
| PbS      | 1.7              |
| BaO      | 0.61             |
| MnO      | 0.53             |
| SrO      | 0.46             |
| TiCl     | 0.36             |
| CsCl     | 0.14             |
| LiF      | 0.08             |

IV. CONCLUSION

To summarize the results from this study, we refer to our previous work \[7\], where it was shown that the zone-center TO vibrational mode effective charge $Z^*$ can be considered to be the key macroscopic parameter of the el-TO-ph coupling strength. As is well-known, the Born effective charges play a fundamental role in determining the lattice-dynamical properties of insulating crystals and are a powerful tool for investigating the dielectric and ferroelectric properties of materials. In particular, they measure the coupling of IR radiation to the optic phonons. In materials where the el-TO-ph coupling is operative, it can be verified by spectroscopy measurements of the IR-active TO mode.

In this paper, we pioneered the application of experimental data to estimate the interband el-TO-ph interaction constants in a number of representative polar compounds. We sustained theoretical arguments \[7\] with numerical calculations of the interband el-TO-ph interaction constants and the further comparative analysis that the large interband el-TO-ph interaction is a special microscopic feature of the ferroelectric materials. Thus, one can conclude that the presence of anomalously large Borns effective charges is the key signature that the interband el-TO-ph coupling is essentially strong in a ferroelectric material. In contrast, in non-ferroelectrics, the strength of the el-TO-ph interaction is not necessarily high enough due to their lower polar nature. This result corresponds to the main assumption of the vibronic theory \[12-15\] regarding the existence of sufficiently strong interband el-TO-ph coupling in displacive ferroelectrics. The strength of the interband el-TO-ph interaction can therefore serve as a direct indicator of the extent to which a crystal lattice is close to a possible ferroelectric instability.

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Figure captions

Fig. 1: Dependence of the square root of the dimensionless el-TO-ph coupling parameter on zone-centre TO vibrational mode effective charge. Triangles shown on the figure are the values of $|Z^*|$ and $\sqrt{\kappa}$ determined separately for each compound. The values of $|Z^*|$ are calculated from the experimental data given in Tables 1 and 2. The direct line is the resulting fit.
