Prediction uncertainty of density functional approximations for properties of crystals with cubic symmetry

Supplementary Material

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We provide here tables of all the data used in the companion paper and tables of the coefficients to estimate the corrected values and prediction uncertainties of the studied methods.

**Validation data.** Tables 1-6.

Reference data were collected for the following crystals (*Strukturbericht* designation\(^1\) in parentheses): 22 semiconductors, also present in the SC40 data set\(^2\), namely: C(A4), Si(A4), Ge(A4), SiC(B3), BN(B3), BP(B3), BAs(B3), AlP(B3), AlAs(B3), AlSb(B3), GaN(B3), GaN(B4), GaP(B3), GaAs(B3), GaSb((B3), InP(B3), InAs(B3), InSb(B3), ZnS(B3), ZnSe(B3), ZnTe(B3), CdTe(B3), MgS(B1); 4 alkali halides: LiF(B1), LiCl(B1), NaF(B1) and NaCl(B1); and, two oxides: MgO(B1), SrTiO\(_3\)(E2\(_1\)).

The reference dataset includes: experimental lattice constant values corrected for the zero-point anharmonic expansion, as reported in Ref.\(^3\); experimental bulk modulus values, taken from Refs.\(^4\)-\(^7\), and low temperature (below 77 K) experimental (fundamental) band gap values\(^2,5,8,9\).

For bulk modulus, we referred to low temperature data\(^4\)-\(^6\), if available, and, when possible, the zero-point anharmonic expansion correction has been included from Ref\(^6\).

The band gaps considered cover two orders of magnitude, between \(\approx 0.2\) and \(\approx 12\) eV.

**Validation data.** Tables 7-10.

A set of 9 systems has been set aside for validation purpose. These systems have been chosen on the basis that we did find reference values for band gaps and lattice constants, but none for bulk moduli: AlN(B3), CdS(B3), CdSe(B3), MgSe(B1), MgTe(B1), BaS(B1), BaSe(B1), BaTe(B1), and LiH(B1).

**Property and uncertainty prediction.** Tables 11-13.

For the estimation of a new value of a property knowing a calculated value \(c_s\) (for a system not in the benchmark set), the prediction model and prediction variance corre-
sponding to the chosen DFA are\textsuperscript{10}

\begin{align*}
p(c_s) &= a + bc_s \quad (1) \\
u_p^2(c_s) &= u_f^2(c_s) + d^2 \quad (2) \\
u_{jm}^2(c_s) &= u^2(a) + u^2(b)c_s^2 + 2u(a, b)c_s. \quad (3)
\end{align*}

For the comparison of a model prediction with reference data, or the prediction of an experimental result, this variance has to be further combined with the corresponding reference/experimental data uncertainty

\[ u^2(c_s) = u_p^2(c_s) + u_s^2. \quad (4) \]

**References**


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Table 9: Validation data for band gaps (eV).

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<td>5.73</td>
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<td>7.98</td>
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Table 11: Calibration and prediction uncertainty parameters for lattice constants (Å).

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<th>w^2(a)</th>
<th>w^2(b)</th>
<th>w(a,b)</th>
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<td>0.001030</td>
<td>0.000038</td>
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</tr>
<tr>
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</tr>
<tr>
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<tr>
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<td>0.961603</td>
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</tr>
<tr>
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<td>0.977020</td>
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### Table 12: Calibration and prediction uncertainty parameters for bulk modulus (GPa).

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<th>$u^2(b)$</th>
<th>$u(a, b)$</th>
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<tr>
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<td>6.27555</td>
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</tr>
<tr>
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<td>1.056710</td>
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<td>5.86778</td>
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<tr>
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<td>61.0518</td>
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</tr>
<tr>
<td>B97</td>
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<td>4.83764</td>
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<tr>
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### Table 13: Calibration and prediction uncertainty parameters for band gaps (eV).

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<th>$u^2(b)$</th>
<th>$u(a, b)$</th>
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<tr>
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