BSSE-corrected consistent Gaussian basis sets of triple-zeta valence with polarization quality of the sixth period for solid-state calculations

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Abstract
Consistent basis sets of triple-zeta valence with polarization quality for the elements Cs-Po were derived for periodic quantum-chemical solid-state calculations. They are an extension of the pob-TZVP-rev2 [Vilela Oliveira, D.; Laun, J.; Peintinger, M. F. and Bredow, T., J. Comput. Chem., 2019, 40 (27), 2364–2376] basis sets and are based on the fully relativistic effective core potentials (ECPs) of the Stuttgart/Cologne group and on the def2-TZVP valence basis of the Ahlrichs group. The basis sets are constructed to minimize the basis set superposition error (BSSE) in crystalline systems. The contraction scheme, the orbital exponents, and contraction coefficients were optimized in order to ensure robust and stable self-consistent-field (SCF) convergence for a set of compounds and metals. For the applied PW1PW hybrid functional, the average deviations of the calculated lattice constants from experimental references are smaller with pob-TZVP-rev2 than with standard basis sets available from the CRYSTAL basis set database.

KEYWORDS
6th period, basis sets, CRYSTAL, pob-TZVP-rev2, solid-state calculations

1 | INTRODUCTION

The precision of quantum-chemical calculations in terms of structural and electronic properties depends on the applied set of basis functions. Most implementations of density functional theory (DFT) and Hartree-Fock (HF) employ either plane-wave basis sets or atom-centered contracted Gaussian basis functions (CGFs). While plane waves are independent of the given element or compound, CGFs are atom-dependent and have to be developed explicitly for each chemical element.

For molecular quantum-chemical calculations, Gaussian-type basis sets at various quality levels are available for almost every element of the periodic table.1-3 For example, the widely used def2 basis sets of the Ahlrichs group are of particular significance as they are implemented in common molecular quantum-chemical codes.4-7 Since these basis sets were generated explicitly for molecular systems, they cannot be directly transferred to CRYSTAL periodic solid-state calculations without further modifications, otherwise this would lead to linear-dependence issues. Other periodic quantum-chemical codes such as the riper module8-11 implemented in the TURBOMOLE program since V7.012 are able to directly employ molecular basis sets to solid-state calculations by a transformation into linear-independent basis sets regardless of the orbital exponents.

Based on the corresponding Ahlrichs def2 basis sets, we developed in previous work consistent Gaussian basis sets of double- and triple-zeta with polarization quality for H–I (pob-DZVP and pob-TZVP)13,14 as well as a revised BSSE-corrected version for H–Br (pob-TZVP-rev2 and pob-DZVP-rev2)15 with the exception of the noble
gases and Tc. The pob-DZVP and pob-TZVP basis sets are well-balanced and generally applicable for solid-state calculations with the widely used crystalline-orbital program CRYSTAL1716,17 and show a better overall performance compared to CRYSTAL standard basis sets.18

In this work, we extend the pob-TZVP-rev2 basis sets to the s-, p-, and d-block elements of the sixth period. Scalar-relativistic effects are implicitly taken into account by using the widely applied effective core potentials (ECPs) of the Stuttgart/Cologne Group19 to represent the core electrons. The valence functions are based on Ahlrichs def2-TZVP. Based on our experience from previous projects,15 we took our BSSE-correction scheme for crystalline solids into account.

The resulting pob-TZVP-rev2 basis sets are obtained in three steps: (1) modification of the contraction scheme, (2) optimization of the outer orbital exponents and contraction coefficients, and (3) applying the BSSE correction. They are evaluated by calculating the lattice constants of selected solid compounds and a comparison to CRYSTAL standard basis sets and experimental data. For the sake of completeness, we also provide a basis set for Po, but it is untested due to lack of experimental references.

2 BASIS SET OPTIMIZATION

The valence shells of the basis sets presented in this work are based on the def2-TZVP basis sets developed by the group of Ahlrichs5 whereas core electrons are replaced by fully relativistic ECPs.19 For every valence shell there is at least one primitive polarization function of higher angular momentum.

For our basis sets we chose the following ECPs of the Stuttgart/Cologne group19 which represent 46 or 60 core electrons for the s- or p- and d-block elements, respectively: Cs,20 Ba,21 Hf,22 Ta, Ta, W,22 Re,23 Os,23 Ir,22 Pt,22 Au,23 Hg,23 Tl,24 Pb,25 Bi,25 Po.26

The following variational optimization procedure is described in detail in previous works.13–15 Starting point is the modification of the contraction scheme by removing all primitive functions with orbital exponents smaller than 0.15. The pob-TZVP-rev2 basis sets retain the highly contracted def2-TZVP shells and are, if necessary, augmented with primitive Gaussians until the number of basis functions matched the triple-zeta with polarization level. In contrast to the molecular def2-TZVP basis sets, we observed that additional contracted s-functions are required for p-block element solid-state calculations. A comparative overview of the contraction scheme for the final pob-TZVP-rev2, the original def2-TZVP and the applied CRYSTAL standard basis sets is given in Table 1.

In the next step, we optimized the outer orbital exponents and contraction coefficients with a lower limit 0.15 for the orbital exponents. This threshold assures numerical stability and provides accurate results at reasonable computational effort. For special cases these resulting basis sets have to be augmented with diffuse functions (see Section 4.3).

In order to estimate the atomic BSSE and to take this effect into account, we calculated the counterpoise correction for every basis set in a selected bulk system applying ATOMBSSE in CRYSTAL17 (see Section 4.4). If necessary, the basis sets were re-optimized in order to minimize counterpoise correction.

In the final step, we performed test calculations for ionic and semiconducting compounds and made further small adjustments to improve the numerical stability. Since the presented optimization procedure is an iterative process, the resulting final basis sets are not fully variational for all reference systems but perform well in the considered range of binding situations at reasonable computational cost and with good SCF stability.

| Element | Number of functions (ECP/s/p/d/f) |
|---------|----------------------------------|
| pob-TZVP-rev2 | def2-TZVP | CRYSTAL |
| Cs | 46/3111/41/1 | 46/31111/411/111 | 46/31/31/1 |
| Ba | 46/2111/411/1 | 46/211111/411/111/1 | 46/31/311/1 |
| Hf | 60/41111/411/311/1 | 60/41111/411/111/1 | 60/411/31/41 |
| Ta | 60/41111/411/311/1 | 60/41111/411/111/1 | 60/31/31/1 |
| W | 60/31111/411/1 | 60/311111/411/111/1 | 68/11/11/31 |
| Re | 60/31111/411/1 | 60/311111/411/111/1 | 68/11/31/1 |
| Os | 60/31111/411/1 | 60/311111/411/111/1 | 60/31/221/1/4 |
| Ir | 60/31111/411/1 | 60/311111/411/111/1 | 60/341/2/147 |
| Pt | 60/31111/411/1 | 60/3111111/411/111/1 | 60/31/2211/41/48 |
| Au | 60/31111/411/1 | 60/3111111/411/111/1 | 60/441/31/21 |
| Hg | 60/31111/411/1 | 60/311111/411/111/1 | 60/441/4|1 |
| Tl | 60/4221/3311/6111 | 60/422111/3311/6111/1 | 68/31/31/1 |
| Pb | 60/4221/3311/6111 | 60/422111/3311/6111/1 | 60/8811/8811/611/1 |
| Bi | 60/4221/3311/6111 | 60/422111/3311/6111/1 | 60/441/41/4153 |
| Po | 60/5221/3411/6111 | 60/5211111/341111/6111/1 | – |

The table shows the number of core electrons which are replaced by the pseudopotential (ECP) and number of contracted basis functions (s/p/d/f) for the pob-TZVP-rev2, def2-TZVP and selected CRYSTAL standard basis sets.

The N-dash indicates that there is no basis set available.

TABLE 1 Number of core electrons which are replaced by the pseudopotential (ECP) and number of contracted basis functions (s/p/d/f) for the pob-TZVP-rev2, def2-TZVP and selected CRYSTAL standard basis sets.
### 3 | COMPUTATIONAL DETAILS

The basis sets and structure optimizations were carried out with the crystalline orbital program CRYSTAL17 version 1.0.2\textsuperscript{16,17} using the hybrid density functional theory (DFT) functional PW1PW\textsuperscript{27} which is based on the PWGGA\textsuperscript{28} functional including 20\% Fock exchange. Previous work has shown that PW1PW provides accurate results for structural parameters of ionic and semiconducting solids.\textsuperscript{14,15,29,30} The basis-set optimizations were accomplished with a python-script, which runs single-point calculations with CRYSTAL17 and uses the numerical minimization library MINUIT.\textsuperscript{31} This procedure has already been used in our previous basis set developments.

The truncation criteria for bi-electronic integrals were set to $10^{-7}$ for the overlap and penetration threshold for the Coulomb integrals, and for the overlap threshold for HF exchange integrals. For the pseudo overlap in the HF exchange series, the truncation criteria were set to $10^{-14}$ and $10^{-42}$ (TOLINTEG 7 7 14 42). The SCF accuracy was set to $10^{-7}$ a.u. for optimizations of geometry for ionic and semiconducting compounds. We used a $8 \times 8 \times 8$ Monkhorst-Pack and Gilat net for the cubic systems and equally dense and balanced grids for the other crystal systems. For the counter-ions we applied our pob-TZVP-rev2 basis sets throughout.

For the geometry optimizations of bare metals and the calculations of corresponding band structures, we decreased the integral thresholds (TOLINTEG 9 9 27 48) and applied a denser $24 \times 24 \times 24$ Monkhorst-Pack grid and a $48 \times 48 \times 48$ Gilat net. In these cases, we additionally used finite-temperature schemes (SMEAR) with 0.01 a.u. width.

To compare our resulting lattice constants for selected cubic compounds on HF level, we approximated the HF-limits using the Vienna (SMEAR) with 0.01 a.u. width. These cases, we additionally used finite-temperature schemes (TOLINTEG 9 9 27 48) and applied a denser $24 \times 24 \times 24$ Monkhorst-Pack grid and a $48 \times 48 \times 48$ Gilat net. In these cases, we additionally used finite-temperature schemes (SMEAR) with 0.01 a.u. width.

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### 4 | RESULTS AND DISCUSSION

For an evaluation of the resulting basis sets, it is necessary to test their stability and transferability. For this purpose, we compared the calculated lattice parameters with pob-TZVP-rev2 and the available CRYSTAL standard basis sets on hybrid DFT and HF level to experimental references. For the transition metals, the electronic band structure was included in the comparison. Even if the measurement of the quality of the basis sets is limited by the underlying theoretical approach, we have shown in previous works that this procedure is sufficient to evaluate the overall performance. Finally, the estimation of the BSSE in crystalline systems is given to show the consistency of the developed basis sets with our previous work.

### 4.1 | Ionic and semiconducting systems

To test our basis sets, we optimized the lattice parameters and atomic positions of selected chalcogenides and halides, which can be classified as ionic compounds and semiconductors. The results are given in Table 2 for cubic, in Table 3 for trigonal and tetragonal, and in Table 4 for orthorhombic and monoclinic systems. Their evaluation in terms of the relative error with respect to experiment is given in Figure 1 for cubic, in Figure 2 for trigonal and tetragonal and in Figure 3 for orthorhombic and monoclinic systems, respectively.

Due to the polymorphism of WO$_3$,\textsuperscript{35,36} we calculated the lattice constants and atomic positions of triclinic WO$_3$,\textsuperscript{37} which should

#### Table 2 Experimental and calculated lattice parameters (Å) of selected ionic cubic solid compounds with pob-TZVP-rev2 and CRYSTAL standard basis sets. RMSD, maximum error, and standard deviation ($\sigma$) of lattice constants with respect to experiment in percent

| Compound | $a$ | $c$ | $\sigma$ | Max. Error |
|----------|-----|-----|---------|------------|
| CsCl     | 4.12 | 4.14 | 1.21 | 2.45 | 0.77 |
| BaO      | 5.54 | 5.55 | 0.72 | 0.72 | 0.27 |
| BaF$_2$  | 6.20 | 6.22 | 0.35 | 0.35 | 0.27 |
| HfN      | 4.52 | 4.52 | 3.74 | 3.74 | 3.73 |
| TaO      | 4.43 | 4.32 | 1.54 | 1.54 | 1.54 |
| ReO$_3$  | 3.75 | 3.75 | 0.51 | 0.51 | 0.51 |
| Os$_2$   | 5.62 | 5.51 | 1.16 | 1.16 | 1.16 |
| Pt$_3$O$_4$ | 5.59 | 5.63 | 3.48 | 3.48 | 3.48 |
| Tl$_2$O$_3$ | 10.54 | 10.62 | 5.11 | 5.11 | 5.11 |
| PbO$_2$  | 5.35 | 5.31 | 2.40 | 2.40 | 2.40 |
| PbS      | 5.94 | 5.95 | 2.45 | 2.45 | 2.45 |
| RMSD     | 0.72 | 0.72 | 0.35 | 0.35 | 0.35 |

#### Table 3 Experimental and calculated lattice parameters (Å) of selected ionic trigonal (Cs$_2$O, HgS) and tetragonal (OsO$_2$, IrO$_2$) solid compounds with pob-TZVP-rev2 and CRYSTAL standard basis sets. The N-dash indicates that the structure optimization failed. RMSD, maximum error, and standard deviation ($\sigma$) of lattice constants with respect to experiment in percent

| Compound | $a$ | $c$ | $\sigma$ | Max. Error |
|----------|-----|-----|---------|------------|
| Cs$_2$O  | 4.26 | 18.99 | 4.24 | 0.51 |
| OsO$_2$  | 4.50 | 3.18 | 4.44 | 1.54 |
| IrO$_2$  | 4.51 | 3.16 | 4.49 | 0.39 |
| HgS      | 4.15 | 9.50 | 4.11 | 0.39 |

| Compound | $a$ | $c$ | $\sigma$ | Max. Error |
|----------|-----|-----|---------|------------|
| RMSD     | 1.21 | 1.21 | 0.51 | 0.51 |
| Max. Error | 3.35 | 3.35 | 1.54 | 1.54 |
| $\sigma$ | 0.81 | 0.81 | 0.39 | 0.39 |
correspond to the low-temperature minimum structure. The results are given in Table S1.

For the given crystal systems, we summarize the root mean square deviation (RMSD), the maximum error, and the standard deviation of the calculated lattice constants for the pob-TZVP-rev2 and CRYSTAL standard basis sets, respectively. For all noncubic systems, the calculated maximum error is the sum of all lattice parameter errors. Our presented basis sets perform well in total, as the RMSD was reduced significantly from 0.75% to 0.38% compared to the standard basis sets in all crystal structures and show a good transferability, as shown by the lower standard deviation of 0.31% in comparison to 0.69%. The SCF stability was improved with respect to the CRYSTAL standard basis sets in all cases.

### 4.2 HF calculations

The accuracy of our pob-TZVP-rev2 basis sets depends on the chosen hybrid PW1PW functional. To assure that the presented basis sets are applicable to other methods, we additionally calculated the

| Compound | Experiment | CRYSTAL | pob-TZVP-rev2 |
|----------|------------|---------|--------------|
|          | a          | b       | c            | β          | a          | b       | c            | β          |
| HfO₂     | 5.12       | 5.18    | 5.29         | 99.22      | 5.12       | 5.19    | 5.26         | 99.15      | 5.11       | 5.16    | 5.27         | 99.36      |
| TaON     | 4.95       | 5.02    | 5.17         | 99.61      | 4.95       | 5.01    | 5.15         | 99.63      | 4.97       | 5.03    | 5.17         | 99.62      |
| ReO₂     | 4.81       | 5.64    | 4.60         | 54.35      | 4.79       | 5.63    | 4.57         | 54.55      | 4.83       | 5.62    | 4.58         | 54.88      |
| IrS₂     | 19.79      | 3.57    | 5.62         | 69.14      | 20.11      | 3.61    | 5.72         | 69.34      | 19.91      | 3.58    | 5.68         | 69.18      |
| PtO₂     | 4.48       | 4.54    | 3.14         | 70.35      | 4.54       | 4.52    | 3.16         | 70.38      | 4.51       | 4.53    | 3.13         | 70.38      |
| Au₂O₃    | 12.83      | 10.52   | 3.84         | 71.35      | 12.85      | 10.55   | 3.89         | 71.39      | 12.83      | 10.48   | 3.82         | 71.38      |
| Bi₂O₃    | 5.83       | 8.14    | 7.48         | 67.07      | 5.95       | 8.12    | 7.45         | 67.03      | 5.87       | 8.11    | 7.47         | 67.88      |
| RMSD     |            |         |              | 0.64       | 0.35       |          |          |              |            | 0.60     | 0.29       |
| Max. Error |          |         |              | 4.40       | 2.36       |          |          |              |            |          |          |

**Table 4** Experimental and calculated lattice parameters (Å, degree) of selected monoclinic (HfO₂, TaON, Bi₂O₃) and orthorhombic (ReO₂, IrS₂, PtO₂, Au₂O₃) solid compounds with pob-TZVP-rev2 and CRYSTAL standard basis sets. RMSD, maximum error, and standard deviation (σ) of lattice constants with respect to experiment in percent.

**Figure 1** Relative error in the lattice constants of cubic compounds with respect to experimental values.
lattice constants for the cubic compounds on HF level. The resulting lattice parameters are given in Table 5 and are evaluated relative to the HF-limit approximately obtained with VASP in Figure 4. In comparison to hybrid DFT calculations, the RMSD increases from 0.72% to 0.82% for the CRYSTAL and from 0.35% to 0.67% for the pob-TZVP-rev2 basis sets, while keeping the numerical stability. Both, the pob-TZVP-rev2 and the CRYSTAL standard basis sets are applicable to HF calculations of solids, which might be a starting point for post-HF methods such as Møller-Plesset perturbation theory for periodic systems.38,39
The quality of the chosen basis sets is particularly critical in the case of metallic systems. To reproduce the nearly uniform valence electron density, the atoms in general need additional diffuse Gaussians compared to ionic systems or semiconductors. Although this augmentation often causes linear-dependency issues, it is strongly recommended in order to obtain accurate structural and electronic results for metallic systems. In line with this recommendation, we added diffuse $s$- and $p$-functions with orbital exponents of $\frac{1}{2}$ to $\frac{3}{4}$ of the next inner orbital exponent, denoted as pob-TZVP-rev2. To assure the stability and transferability of our basis sets, we do not include these functions in the presented basis sets and suggest the augmentation for bulk or surface calculations of metals.
The optimized lattice parameters obtained with pob-TZVPD-rev2 are compared to those with CRYSTAL standard basis sets in Table 6. Inspection shows a RMSD of 0.37% for the pob-TZVPD-rev2 lattice constants, confirming the quality of the presented basis sets.

An additional evaluation of our basis sets is made by calculating the band structures of the given metals in comparison to those obtained with VASP. To eliminate the influence of the functional, geometry optimization and band structure calculations were performed with the PBE functional, respectively. We applied the k-vector path recommended by Curtarolo et al.40 to cover all special k-vector points of the asymmetric unit.

The resulting band structures of gold are given in Figure 5, for all other elements they can be found in Table 2 and Figures S1–S9. The pob-TZVPD-rev2 and the plane wave VASP band structures are similar, especially for the special k-vector points, which shows the quality and transferability of our presented basis sets in the framework of metallic systems.

### 4.4 BSSE in crystalline systems

In previous work, we have noticed that some pob basis sets strongly suffer from the BSSE.15 Therefore, we took the atomic BSSE in crystalline systems into account by calculating the counterpoise energy via CRYSTALS ATOMBSSE. The results are given in Figure 6. The unreasonably high atomic BSSE of 3759 kJ/mol for the CRYSTAL Os basis set cannot be explained and is not included in the statistics. The averaged atomic BSSEs are 157 kJ/mol (pob-TZVPD-rev2) and 336 kJ/mol (CRYSTAL). Although BSSE is slightly larger in certain cases with the pob-TZVPD-rev2 compared to CRYSTAL standard basis

| Metal | Experiment | CRYSTAL | pob-TZVPD-rev2 |
|-------|------------|---------|---------------|
|       | A          | c       | a             | c           | Shell (Exponent) |
| Hf    | 3.20       | 5.06    | 2.9879        | 4.78        | s (0.05), p (0.10) |
| Ta    | 3.31       |         | 2.8946        |             | s (0.10) |
| W     | 3.16       |         | 3.0421        |             | p (0.15) |
| Re    | 2.76       | 4.46    | 2.7276        | 4.24        |             |
| Os    | 2.74       | 4.32    | 2.3760        | 3.79        | p (0.12) |
| Ir    | 3.84       |         | 3.8777        |             | p (0.10) |
| Pt    | 3.92       |         | 3.9848        |             |             |
| Au    | 4.08       |         | 4.0669        |             | s (0.10) |
| Tl    | 3.88       |         | 4.0451        |             | s (0.10) |
| Pb    | 4.95       |         | 4.8652        |             |             |

The optimized lattice parameters obtained with pob-TZVPD-rev2 are compared to those with CRYSTAL standard basis sets in Table 6. Inspection shows a RMSD of 0.37% for the pob-TZVPD-rev2 lattice constants, confirming the quality of the presented basis sets.
sets (Ir, Pt, Au, Tl, Bi), it is much more consistent throughout the period. This is evident from the standard deviation of 302 kJ/mol with CRYSTAL and 36 kJ/mol with pob-TZVP-rev2.

5 | CONCLUSIONS

We have presented well-balanced BSSE-corrected and generally-applicable basis sets of consistent TZVP level for the elements of the sixth period for quantum-chemical solid-state LCAO calculations. These basis sets are an extension of our previously developed pob-TZVP-rev2 series and are characterized by high numerical stability and accurate geometry optimizations for a range of different ionic and semiconducting compounds and bare metals. We have shown that the accuracy of the calculated lattice parameters is improved over the standard basis sets provided by the CRYSTAL database, which applies both on hybrid DFT and on HF level. All basis sets are available for download with neutral atomic configurations from our website (https://www.chemie.uni-bonn.de/pctc/mulliken-center) and as Supporting Information to this article.

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DATA AVAILABILITY STATEMENT

All basis sets are available for download with neutral atomic configurations from our website (https://www.chemie.uni-bonn.de/pctc/mulliken-center) and as Supporting Information to this article. The data that support the findings of this study are available from the corresponding author upon reasonable request.

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