Abstract

Hybrid density functional (HDF) approximations usually deliver higher accuracy than local and semilocal approximations to the exchange-correlation functional, but this comes with drastically increased computational cost. Practical implementations of HDFs inevitably involve numerical approximations – even more so than their local and semilocal counterparts due to the additional numerical complexity arising from treating the exact-exchange component. This raises the question regarding the reproducibility of the HDF results yielded by different implementations. In this work, we benchmark the numerical precision of four independent implementations of the popular Heyd-Scuseria-Ernzerhof (HSE) range-separated HDF on describing key materials’ properties, including both properties derived from equations of states (EOS) and band gaps of 20 crystalline solids. We find that the energy band gaps obtained by the four codes agree with each other rather satisfactorily. However, for lattice constants and
bulk moduli, the deviations between the results computed by different codes are of the same order of magnitude as the deviations between the computational and experimental results. On the one hand, this means that the HSE functional is rather accurate for describing the cohesive properties of simple insulating solids. On the other hand, this also suggests that the numerical precision achieved with current major HSE implementation is not sufficiently high to unambiguously assess the physical accuracy of HDFs. It is found that the pseudopotential treatment of the core electrons is a major factor that contributes to this uncertainty.

Introduction

The reproducibility of the results, both experimental and computational ones, is essential for scientific researches. In computational materials science which heavily relies on computer simulations, this is particularly a concern. Ideally, one would like to see that the same results be obtained regardless which computer code is used. As one of the most widely used first-principles approaches for simulating materials’ properties, the generalized gradient approximations (GGAs) in density functional theory (DFT), such as the Perdew-Burke-Ernzerhof (PBE)\textsuperscript{1} functional, have been implemented in a plethora of computer codes and widely applied in condensed physics, quantum chemistry, and materials science. A natural question arises regarding the reproducibility of the GGA results as obtained by different computer codes. This question was addressed by Lejaeghere \textit{et al.} in Ref. \textsuperscript{2} where the reproducibility of the PBE implementations has been examined over 15 different computer codes, using 40 different potentials and/or basis set types, for describing the equation of states (EOS) of 71 elemental crystals. These authors introduced a so-called $\Delta$ gauge - a single value that measures the deviations of the EOS curves yielded by two different codes – and found that the $\Delta$ values between mainstream DFT codes, averaged over the elemental crystals, are at the level of 1 meV. Such a remarkable numerical precision assures the reproducibility of the mainstream DFT codes, as far as the PBE functional concerned.
In recent years, the hybrid density functionals (HDFs) are getting more and more popular in computational materials science. By incorporating a fraction of Hartree-Fock exchange (HFX), HDFs successfully addressed one big issue of local-density approximation (LDA) and GGA-type functionals – the severe underestimation of the band gaps of semiconductors and insulators. Popular HDFs include B3LYP, PBE0 and HSE. Among these, the HSE functional belongs to the screened HDFs in which the Coulomb interaction is split into short-range and long-range components and only the HFX based on the short-range Coulomb interaction is mixed into the exchange-correlation (XC) functionals. Incorporating the HFX only for the short-range part of the Coulomb interaction is arguably better suited for describing narrow- and middle-gap semiconductors than global HDFs. In practice, the HSE functional shows remarkable performance not only for band gaps, but also for structural and cohesive properties. The price to pay, however, is the significantly increased computational cost, arising from the evaluation of the short-range HFX, compared to GGAs.

Nowadays, HDFs have been implemented in various mainstream first-principles code packages, employing different potentials, basis sets, and numerical approximations. For example, in the Vienna Ab initio Simulation Package (VASP), the HFX is computed within the projector augmented wave (PAW) formalism and plane-wave (PW) basis set. The VASP implementation reduces the computational cost by downsampling the k-point grid in the HFX evaluations. As for atomic-orbital based codes, the resolution-of-the-identity (RI) is often employed to reduce the computational cost of HFX component. In particular, using the localized variant of the RI approximation, one can achieve a linear scaling of the computational cost for building the HFX matrix with respect to the system size \( N \). The localized RI (LRI) based HDFs have been implemented within the Fritz Haber Institute ab initio molecular simulations (FHI-aims) code package and recently also in the atomic-orbital-based ab initio computation at UStc (ABACUS) code package. Besides these efforts, Lin developed an adaptively compressed exchange operator (ACE) scheme, which, together with a two-level self-consistent field iterator procedure, can significantly
accelerate the HDF calculations using PW basis sets. Such a scheme has been implemented in the DGDFT \cite{30,31} and the Quantum ESPRESSO (QE) \cite{32,33} code packages. Other techniques to speed up the HFX calculations include the exploration of the localization offered by Wannier representation \cite{34,35,36}, interpolative separable density fitting approaches \cite{37,38} and representing NAOs in terms of Gaussian-type orbitals \cite{39} etc.

As alluded to above, the numerical precision and the reproducibility of PBE implementations in mainstream DFT codes have been established via the \( \Delta \)-value project. However, this conclusion may not be automatically extended to HDFs as implemented in these codes. In fact, the numerical precision of HDF calculations does not only rely on the treatment of electron-ion interactions (pseudopotentials vs. all-electron) and basis set types (e.g., plane waves vs. atomic orbitals), but also on the numerical approximations involved in the evaluation of the HFX potential and energy. To our knowledge, a systematic assessment of the numerical precision of different HDF implementations has not yet been reported. In this work, utilizing the HSE functional available in four computer codes, including VASP, FHI-aims, QE, and ABACUS, whose HDF implementations differ considerably in algorithmic and numerical details, we assess the reproducibility of HSE results by computing the pairwise \( \Delta \) values among these four codes, based on the energy-volume curves of 20 binary compounds. These 20 compounds have been widely used as a test set for evaluating the performance of HDFs \cite{9,24,41,42,43,44}. Such a \( \Delta \)-value based assessment will be corroborated by additional properties including the lattice constants, bulk moduli, and band gaps. Naturally, benchmarking the numerical precision of HDF implementations over all mainstream DFT codes and across different types of materials requires community-wide efforts and goes beyond the scope of the present paper. Nevertheless our work provides a solid basis that will hopefully stimulate more benchmark efforts in this direction.

4
Methods

In this section, we recapitulate the essentials of the numerical frameworks and computational setups employed in the four codes considered in this work. First of all, different strategies are used to treat the effects arising from the nuclei and core electrons: The VASP code employs the PAW method whereas QE and ABACUS make use of the SG15 optimized norm-conserving Vanderbilt-type (ONCV) pseudopotentials.\textsuperscript{15,16} In contrast, FHI-aims treats all electrons on an equal footing. Scalar relativistic effects are included either in the PAW or norm-conversing pseudopotentials (NCPP), or via the “atomic ZORA” scheme\textsuperscript{17,18} in the all-electron case. The spin-orbit coupling effect is not included in the HSE calculations here.

Regarding the basis sets, VASP and QE both use PWs to expand the Bloch wavefunctions, whereas numerical atomic orbital (NAO) basis sets are used in the FHI-aims and ABACUS codes, although different NAO construction strategies are adopted in these two codes, in order to best represent their respective all-electron (AE) or pseudo-wavefunctions. Moreover, kinetic energy cutoffs of 550 eV and 100 Rydberg (Ry) are used for the PW expansion of wavefunctions in VASP and QE calculations, respectively. For FHI-aims, the default “tight” NAO basis sets\textsuperscript{26} are adopted, whereas the so-called “DZP-DPSI”\textsuperscript{49} basis sets are employed in ABACUS. Additionally, 100 Ry energy cutoff is used in ABACUS for the Hartree potential calculation and for determining the uniform quadrature grid. In Table I, we summarize the computational settings for the four codes, together with the convergence thresholds in the self-consistent calculations. Please note that these settings are roughly the default ones that are typically used in production calculations. Our intention here is not to push towards the limit of high-precision settings of each code, but rather to check the numerical precision that is achieved in routine calculations. An investigation of the influence of difficult levels of basis sets and numerical settings on the achieved precision of the results has recently been reported by Carbogno et al\textsuperscript{50} for three different computer codes, including FHI-aims.

As mentioned above, additional complexity is involved in the evaluation of the HFX component of the HDFs. For VASP, the standard HSE implementation as available in VASP
5.4.1 is used. As for QE calculations, we use its PWSCF module v.6.5 where the ACE technique is used as the default to calculate the HFX contributions. Finally, for NAO-based codes, the LRI approximation is used in both FHI-aims and ABACUS for evaluating the HFX term. To render the numerical errors associated with LRI sufficiently small, an enhanced auxiliary basis set has to constructed, compared to conventional global Coulomb-metric based RI scheme. In FHI-aims, this is achieved by adding a hydrogen-like $5\, g$ function with an effective nuclear charge $Z = 6$ for each element that is solely used to generate extra auxiliary basis functions (ABFs). In ABACUS, additional optimized ABFs can be included to complement the “on-site” ones to increase the numerical accuracy. Furthermore, an efficient pre-screening procedure is invoked to filter out negligibly small contributions to achieve a linear-scaling build of the HFX. The settings of the ABF basis sets, and the pre-screening parameters for ABACUS HSE calculations are given in the Supporting Information (SI) (cf. Table S1 and discussions therein).

The equilibrium volume $V_0$ and bulk modulus $B_0$ of each solid are determined via the Birch–Murnaghan EOS. Since our test set of materials only comprises fcc crystals, the lattice constants $a_0$ is found from the equilibrium volume $V_0$ via $a_0 = (4V_0)^{1/3}$. The $\Delta$ value for a material $\alpha$ between any two codes are obtained from the calculated EOS curves, following the procedure proposed in Ref. For a more trustworthy comparison between experimental cohesive properties and the HSE predictions, the zero-point motion (ZPM) effects are taken into account, utilizing the values as estimated in Ref. for all calculations. Finally, the band gaps are estimated on a discrete $8\times8\times8\, k$-point mesh, and the experimental lattice parameters are used for all the band structure calculations.
Table 1: Numerical frameworks and computational settings for the four codes included in the present benchmark studies. “Method” describes how the effects from the nuclei and core electrons are treated. “Basis sets” tell the type of basis functions to expand the wavefunctions. $E_{\text{cutoff}}$: the kinetic energy cutoffs for the PW expansions (in case of VASP and QE), and for the Hartree potential calculation and for determining the uniform quadrature grid (in case of ABACUS). $\eta_{\text{etot}}$, $\eta_{\rho}$ denotes the convergence threshold for the self-consistency cycle, based on the criteria of total energy, charge density, respectively. (n/a: this metric is not used in the particular code or not set in this benchmark test).

| Method     | Basis sets              | $E_{\text{cutoff}}$ | $\eta_{\text{etot}}$ | $\eta_{\rho}$ |
|------------|------------------------|---------------------|----------------------|---------------|
| VASP       | PAW                    | PW                  | 550 (eV)             | $10^{-6}$ (eV) | n/a           |
| FHI-aims   | AE                     | NAO (tight)         | n/a                  | n/a           | $10^{-6}$     |
| QE         | NCPP$^a$               | PW                  | 100 (Ry)             | $10^{-6}$ (a.u) | n/a           |
| ABACUS     | NCPP$^a$               | NAO (DZP-DPSI)      | 100 (Ry)             | n/a           | $10^{-8}$     |

$a$: the scalar-relativistic SG15 optimized norm-conserving Vanderbilt-type (ONCV) pseudopotentials [24,25].

Results

Equation of states

We start by examining the pairwise $\Delta$ values evaluated in between the four codes, given by an average of the individual $\Delta$ values for the 20 materials. Namely,

$$\Delta_{ij} = \frac{1}{20} \sum_{\alpha=1}^{20} \Delta_{ij}(\alpha)$$  \hspace{1cm} (1)

where

$$\Delta_{ij}(\alpha) = \sqrt{\int_{0.94V_{0,\alpha}}^{1.06V_{0,\alpha}} [E_{i,\alpha}(V) - E_{j,\alpha}(V)]^2 dV / 0.12V_{0,\alpha}}$$  \hspace{1cm} (2)

measures the root-mean-square difference between the energy-volume ($E$-$V$) curves (with aligned energy minima) generated by two codes $i$ and $j$ for a material $\alpha$ in the test set. In Eq. (2), $V_{0,\alpha}$ is the averaged equilibrium volume of the $\alpha$-th material, as predicted by the two codes. A change of the volume within a range of $-6\%$ to $6\%$ around the equilibrium point...
is included in the evaluation of the $\Delta$ value. The thus determined $4 \times 4$ $\Delta$ matrix is shown in Figure 1 for both the PBE and HSE functionals. From Figure 1 one can immediately see that the $\Delta$ values for the HSE functional (right panel) are 2 to 3 times larger than their counterparts for the PBE functional (left panel). This is not entirely surprising since, as mentioned above, additional numerical approximations are involved in the evaluation of the HFX component of the HSE functional and this will very likely yield additional numerical discrepancies between different implementations. Among the four codes, the smallest $\Delta$ value for the HSE functional, 1.7 meV/atom, is obtained between the all-electron FHI-aims code and the PAW-based VASP code, whereas the largest $\Delta$ value, 5.3 meV/atom, occurs between VASP and QE. Although VASP and QE both use the PW basis sets, the norm-conserving pseudopotentials (NCPPs) are used in QE whereas the PAW scheme is used in VASP. The $\Delta$ matrix in Figure 1 suggests that the approach to describe the valence-ion interactions, has a bigger influence than the choice of basis sets. Indeed, a $\Delta$ value of 3.7 meV/atom is obtained between the two NCPP-based codes – QE and ABACUS, which is smaller than the discrepancy between the two PW-based codes (5.3 meV/atom) and between the two NAO-based codes (4.9 meV/atom). Comparing the two panels in Figure 1 one can see that the distribution pattern of the $\Delta$ values among the four codes are rather similar for the PBE and HSE functionals, except that the $\Delta$ values are 2-3 times larger for the HSE functionals, and that the discrepancy between VASP and QE results is less pronounced for the PBE functional. The reason that the two PW-based codes show larger deviations for the HSE functional, while it is much less so for the PBE functional, is probably because the PAWs and NCPPs used in the present calculations are constructed for the PBE functional and not for the HSE functional. It is not fully clear yet whether the ACE approach, that is used in QE calculations, plays any role here.

Next we check how the lattice constants determined by the four HSE implementations agree with one another. In this case, the experimental values are also included for comparison. In Figure 2a we present the pairwise mean absolute deviations (MADs) between the
|       | VASP     | FHI-aims | ABACUS | QE       |
|-------|----------|----------|--------|----------|
| VASP  | 0.0000   | 0.8670   | 2.2795 | 1.1975   |
| FHI-aims | 0.8670   | 0.0000   | 1.8510 | 0.5730   |
| ABACUS | 2.2795   | 1.8510   | 0.0000 | 1.8305   |
| QE    | 1.1975   | 0.5730   | 1.8305 | 0.0000   |

|       | VASP     | FHI-aims | ABACUS | QE       |
|-------|----------|----------|--------|----------|
| VASP  | 0.0000   | 1.7285   | 4.9315 | 5.2595   |
| FHI-aims | 1.7285   | 0.0000   | 4.1070 | 5.1540   |
| ABACUS | 4.9315   | 4.1070   | 0.0000 | 3.7060   |
| QE    | 5.2595   | 5.1540   | 3.7060 | 0.0000   |

Figure 1: The ∆-value matrix (in meV/atom) that measures the pair-wise deviations between the EOS curves generated by four codes, i.e., VASP, FHI-aims, ABACUS, and QE for both PBE (left) and HSE (right) functionals.
four sets of computational HSE lattice constants, as well as those between the computational and experimental results. Specifically, what is presented in Figure 2a are

\[ \text{MAD}(a_0, i, j) = \frac{1}{20} \sum_{\alpha=1}^{20} |a_{0,i}(\alpha) - a_{0,j}(\alpha)| \] (3)

where \(a_{0,i}(\alpha)\) is the equilibrium lattice constant for the \(\alpha\)-th material as determined by experiment \((i = 1)\) or by one of the four HSE implementations \((2 \leq i \leq 5)\). Here, the computational lattice constants are corrected for the ZPM effect. For simplicity, we have assumed that the ZPM corrections are not sensitive to the HSE implementations, and the same ZPM correction values for the HSE lattice constants, as reported in from Ref. 44 (obtained using FHI-aims), are used here for all the computed results. As such, the MADs between the computational results are not affected by the ZPM corrections, and only those between experimental and computational ones are. From Figure 2a one can clearly see that the computational results fall into two groups, i.e., VASP and FHI-aims in one group, and ABACUS and QE in another, with the MADs between the codes within the same group about a factor of 2 smaller than those between the two groups. This again shows, consistent with the \(\Delta\) test, that the all-electron and PAW results agree best, whereas larger deviations of the all-electron/PAW results from the NCPP-based results are observed. As far as the all-electron/PAW results concerned, the deviations between the calculated results are appreciably smaller than the deviations between the computational and experimental results. However, this does not hold any more when all four sets of computational results are taken into account. Finally, one can see that VASP and FHI-aims results show larger deviations from the experimental results than the ABACUS and QE results do. This probably comes from fortuitous error cancellations.

To have a closer look at what is happening behind, in Figure 2b we further present the deviations of the computed lattice constants from the experimental values for the 20 individual compounds. The actual values of the computational and experimental lattice constants
are further presented in Table S2 of SI. Figure 2b shows the VASP and FHI-aims results follow each other closely, whereas QE and ABACUS results show a similar zigzag pattern as the deviations vary among different materials. Such behavior is consistent with the pairwise MAD analysis presented in Figure 2a but Figure 2b also reveals important details. Although for a large part of materials, the four codes yield similar HSE lattice constants, but exceptions do exist. For example, for GaSb, FHI-aims and VASP predict that HSE overestimates the lattice constant by 0.08 Å, whereas QE suggests there is an underestimation of 0.04 Å. Finally, ABACUS yields a HSE lattice constant there is in excellent, but most likely fortuitous agreement with experiment. Similar phenomenon is observed for AlSb whereby VASP and FHI-aims still show a pronounced overestimation, but in this case the HSE lattice constant from QE is in best agreement with experiment, whereas ABACUS shows a slight overestimation. This benchmark test tells that, for some materials, the current HSE implementations may yield appreciably different results than may change the direction of the error when compared to experiment. The way to describe the interactions between valence electrons and ion cores (all-electron, PAW, or NCPPs) seems to play a major role in affecting the outcomes of HSE calculations.

We then perform a similar analysis of the bulk moduli for the same set of compounds, based on the EOS curves generated by the four codes. In Figure 3a, we present the pair-wise MAD matrix for the experimental and four sets of computed HSE bulk moduli. Again the ZPM corrections to the computed bulk moduli are included, using the values reported in Ref. From Figure 3a, we see that the computed results also fall into two groups, with the all-electron FHI-aims and PAW-based VASP results coming closer, and so do the NCPP-based ABACUS and QE results. Between the two groups, we see that the MAD between the two sets of NAO-based results is smaller than that between the PW-based results. Moreover, Figure 3a also reveals that the all-electron/PAW based HSE results show larger deviation from experimental results than the NCPP-based results, similar to the lattice constant case. In Figure 3b, we further present the deviations of the four sets of computed HSE bulk moduli
Figure 2: (a) The pairwise MADs between the computed HSE lattice constants (in Å) by VASP, FHI-aims, ABACUS, QE, and between the computational and experimental values. The colormap is such that the darker the color, the greater the MADs. (b) Deviations between the four sets of HSE lattice constants and the experimental value for individual compounds. The computational lattice constants are corrected for the ZPM effects in both (a) and (b).
from the experimental values for individual materials. The actual values of the HSE bulk moduli as calculated by the four codes, as well as the experimental ones, are presented in Table S3 of SI, for completeness. Here, although the general better agreements between VASP and FHI-aims results, and between the ABACUS and QE results are observable, exceptions do exist. For example, for ZnTe and MgO, the VASP results deviate noticeably from the other three results, whereas the same occurs for the ABACUS results in case of SiC. Despite these discrepancy, some general features can be drawn from this benchmark study. For example, all four codes predict that the HSE bulk moduli of C and BN are appreciably larger than the experimental value, pointing to an intrinsic accuracy limitation of HSE for these hard materials.

**Band gaps**

One important success of the HSE functional is that it significantly improves over local and semi-local functionals for describing the band gaps of semiconductors and insulators, thanks to the HFX component and the generalized KS framework. Thus, the reproducibility of the calculated HSE band gaps is also an important aspect to check, in addition to the EOS-based properties. In Figure 4a, we present the MAD matrix for the band gaps, including the experimental and four sets of HSE results. The actual values of the HSE band gaps, as given by the four codes, as well as the experimental results are presented in Table S4 of the SI. Here, the ZPM contributions to the experimental band gap values are discounted, to facilitate their comparison to computational results (see SI for further details). Here, we clearly see that the MADs between the experimental and computational results are one order of magnitude larger than those between the computational results. This means that, as far as the band gap concerned, the numerical precision of the major HSE implementation is sufficiently high for unambiguously assessing the intrinsic accuracy of the HSE functional. Among the four sets of computational results, the MAD between VASP and FHI-aims results is the smallest, followed by that between FHI-aims and ABACUS. Comparatively, the QE results show
Figure 3: (a) The pairwise MADs between the computed HSE bulk moduli (in GPa) by the four codes, and between the computational and experimental values. The colormap is such that the darker the color, the greater the MADs. (b) Deviations between the four sets of HSE bulk moduli and the experimental value for individual compounds. The computational bulk moduli are corrected for the ZPM effects in both (a) and (b).
larger deviations from those of the other three codes. The closer agreement between the NCPP-based ABACUS and QE results for EOS-derived quantities does not hold anymore for band gaps. Figure 4b further shows the deviations of the four sets of calculated HSE band gaps from the experimental values for individual compounds. Here, one can see that the computational results agree with one another well in general, making them overall clearly separated from the experimental ones. However, there are a few compounds where larger discrepancies are noticeable. These are MgO where the HSE gap by QE shows a deviation as large as 0.5 eV from the results by other codes, followed by InP where a 0.2 eV discrepancy is noticeable. For AlSb, the VASP and FHI-aims gap values show good agreement with experiment, whereas ABACUS and QE results overestimate by the band gap by about 0.4 eV.

Conclusions

In this work, we examined the reproducibility of HSE calculations based on four different implementations in the VASP, FHI-aims, QE, and ABACUS codes, in terms of a test set comprising 20 semiconductors and insulators. These implementations are representative ones as different procedures for treating the core-valence interactions (all-electron, PAW, and NCPP schemes) and different basis sets (PWs and atomic orbitals), with their different combinations, are used. The quantities that we have checked include the $\Delta$ metric as introduced in Ref. 40 as well as the lattice constants, bulk moduli, and the band gaps. We found that, for band gaps, the deviations between the four different sets of computational results are nearly one order of magnitude smaller than the difference between the computational and experimental results. For the EOS-derived properties, e.g., the lattice constants and bulk moduli, the differences between computational and experimental results and those between the computational results themselves, are at the same order of magnitude. On the one hand, this shows the rather good performance of the HSE functional for describing the EOS-derived
Figure 4: (a) The pairwise MADs between the calculated HSE band gaps (in eV) by the four codes, and between the computational and experimental gap results. (b) Deviations between the four sets of HSE band gaps and the experimental value for individual compounds. The ZPM contributions to the experimental band gaps are removed here.
properties; on the other hand, this also means that the numerical precision of HSE implementation still needs to be improved to unambiguously assess its intrinsic accuracy with respect to experimental reference data. Among the computational results, it seems that the prescription for describing the ion-cores plays a significant role in determining the numerical precision of the HSE implementations. Specifically, the all-electron (FHI-aims) and PAW-based (VASP) implementations show better agreement with each other, and so does the NCPP-based implementations (QE and ABACUS), whereas the deviations between these two sets of results are noticeably larger. Nowadays, most NCPP-based HSE calculations are performed using the PBE pseudopotentials. Our work indicates that it is not ideal if high-precision results are aimed for. In principle, one can reduce the core radius and increase the energy cutoffs for NCPP-based calculations to approach the precision of all-electron calculations. However, the computational cost will get exceedingly high to do so. Designing improved NCPPs for HSE and other types of HDF calculations would be a better strategy for improving the quality of NCPP-based HDF calculations. Yang et al. have shown that using the PBE0 pseudopotentials in PBE0 calculations improves the agreement with all-electron calculations for structural parameters and band gaps of some small molecules and simple solids.\textsuperscript{[52]} We expect that this will also holds for the HSE functional and the benchmark set presented in this work.

As HDF calculations get increasingly popular in computational materials sciences, the reproducibility of this type of calculations becomes a prominent issue. Our benchmark calculations in this work only cover a limited set of codes and materials, yet interesting features and trends have been revealed. We hope that this work will stimulate more comprehensive investigations along this line.

Supporting Information Available

The Supporting Information is available free of charge.
• Description of the computational parameters used in ABACUS calculations, and tables containing the computational and experimental values of lattice constants, bulk moduli, and band gaps for 20 solids.

Data availability

All output files of the calculations using VASP, FHI-aims, and QE reported in this work have been uploaded to the NOMAD repository, and can be found, respectively, under the links

https://nomad-lab.eu/prod/v1/gui/user/uploads/upload/id/3WA4ETfQ5bQxPSecuOOPo6kMSQ,
https://nomad-lab.eu/prod/v1/gui/user/uploads/upload/id/CxYC8UV7Rv7EP1FXhrgKw,
https://nomad-lab.eu/prod/v1/gui/user/uploads/upload/id/1I_V_-9Ir_WfKrXiTfsF0Fw.

The input and output files of ABACUS calculations are available from the authors upon reasonable request.

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Graphical TOC Entry

|            | PAW/PW | AE/NAO | NCPP/NAO | NCPP/PW |
|------------|--------|--------|----------|---------|
| PAW/PW     | 0.000  | 1.728  | 4.931    | 5.260   |
| AE/NAO     | 1.728  | 0.000  | 4.107    | 5.154   |
| NCPP/NAO   | 4.931  | 4.107  | 0.000    | 3.706   |
| NCPP/PW    | 5.260  | 5.154  | 3.706    | 0.000   |

\(d^{\text{HSE}}\) (meV/atom)

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