Reproducibility in high-throughput density functional theory: a comparison of AFLow, Materials Project, and OQMD

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A central challenge in high throughput density functional theory (HT-DFT) calculations is selecting a combination of input parameters and post-processing techniques that can be used across all materials classes, while also managing accuracy-cost tradeoffs. To investigate the effects of these parameter choices, we consolidate three large HT-DFT databases: Automatic-Flow (AFlow), the Materials Project (MP), and the Open Quantum Materials Database (OQMD), and compare reported properties across each pair of databases for materials calculated using the same initial crystal structure. We find that HT-DFT formation energies and volumes are generally more reproducible than band gaps and total magnetizations; for instance, a notable fraction of records disagree on whether a material is metallic (up to 7%) or magnetic (up to 15%). The variance between calculated properties is as high as 0.105 eV/atom (median relative absolute difference, or MRAD, of 4%) for formation energy, 0.65 Å³/atom (MRAD of 4%) for volume, 0.21 eV (MRAD of 9%) for band gap, and 0.15 µB/formula unit (MRAD of 8%) for total magnetization, comparable to the differences between DFT and experiment. We trace some of the larger discrepancies to choices involving pseudopotentials, the DFT + U formalism, and elemental reference states, and argue that further standardization of HT-DFT would be beneficial to reproducibility.

Keywords: HT-DFT, MGI, reproducibility, uncertainty, informatics

I. INTRODUCTION

Over the past decade, high-throughput (HT) density functional theory (DFT) has emerged as a widely-used tool for materials discovery and design1–3. In a standard HT-DFT workflow, software tools automate the process of calculating materials properties of interest within DFT, including submitting jobs to high-performance computing infrastructure, on-the-fly error handling, post-processing and dissemination of results, and so on, enabling researchers to evaluate typically 10³–10⁶ materials with minimal human intervention. The resulting database can then be screened for candidate materials exhibiting promising combinations of calculated properties or to search for trends amongst materials behavior to gain new physical insights or develop surrogate models.

The increasingly widespread usage of HT-DFT in materials research can be attributed to a combination of three key factors. First, a large number of specialized codes implement fully automated calculations of specific materials properties within DFT, ranging from phonon dispersions to dielectric tensors. For example, VASP 5,14,5 introduced a feature enabling users to calculate elastic tensors by simply setting a parameter in the input file. Second, the ongoing growth of computing power has ensured that HT-DFT is now well within reach of a single university research group. Third, sophisticated, free, often open-source, software are readily available for managing large numbers of DFT calculations, post-processing output, and storing the resulting data systematically in databases. Thus, a number of HT-DFT databases with various focus areas have emerged; a list of exemplars, including any supporting workflow automation software, is given in Section I of the Supplementary Information.

However, the entirely-automated nature of HT-DFT introduces a few key challenges. First, by definition, the volume of data from HT-DFT is too high for each individual calculation to undergo manual review or analysis.1 How, then, are the quality and integrity of calculations monitored in high-throughput? Second, HT-DFT requires choosing, often at the outset, settings that are consistent across all calculations, encompassing all materials classes and properties being calculated. For example, it may not be known a priori whether the material being calculated is a metal or an insulator. As a result, the calculation parameters that affect, e.g., how electronic occupancies are smeared near the Fermi level must be chosen so that they are applicable to both metals and insulators. Third, practical HT-DFT calculations involve balancing accuracy and computational cost; best-practice recommendations6 involve steps such as explicit convergence tests, which become computationally infeasible in the HT context.

Since HT-DFT has become increasingly central to materials informatics efforts across the spectrum, from high-throughput screening to machine learning7,8 it is crucial to resolve the following concerns: (a) There is no one “correct” solution to some of the challenges of HT-DFT mentioned above, and different databases have tackled them slightly differently. How sensitive are the calculated materials properties to the different HT-DFT parameter choices? (b) The focus areas of many prominent HT-
DFT databases in terms of the materials and properties calculated are often quite different. How interoperable are these various calculated materials properties across HT-DFT databases? We emphasize that such a comparison across HT-DFT databases is different from analyzing the reproducibility of DFT across software implementations and potentials, e.g., focusing on equations of state of elemental crystals\(^9\): the challenges of HT-DFT lie in choosing parameters that are applicable across a wide variety of materials and properties, targeting both reasonable accuracy and computational cost—very distinct from performing highly-accurate DFT calculations of a small set of materials.

Here, we analyze the reproducibility and interoperability of HT-DFT calculations, and demonstrate the benefits of centralizing multiple HT-DFT databases onto a single platform. We critically compare the agreement between three databases for four properties: formation energy (\(\Delta E_f\), volume (\(V\)), band gap (\(E_g\)), and total magnetization (\(M\)). We find certain properties (formation energies and volumes) to be more consistent across databases than others (band gap and magnetization). We then quantify the variability in each of the properties across databases and find that the typical differences between two HT-DFT databases are similar to those between DFT and experiment. Finally, we compare properties across different materials classes to identify characteristics of materials and/or properties that are harder than others to reproduce. In all cases, we identify trends, surface outliers, and investigate potential causes for an observed systematic differences between the databases.

II. METHODS

We focus on three prominent HT-DFT databases in this work: Automatic FLOW (AFLOW)\(^10\), the Materials Project (MP)\(^11\), and the Open Quantum Materials Database (OQMD)\(^3,12\). All three databases contain calculations of a large number of mostly-experimentally reported, ordered compounds from the Inorganic Crystal Structure Database (ICSD)\(^13\). In addition, they contain calculations of many thousands of hypothetical compounds generated from common structural prototypes or other informatics approaches. We note here that all three databases use the VASP software package\(^4,15\) and projector augmented wave (PAW) potentials\(^14,15\) with the Perdew-Burke-Ernzerhof (PBE) parameterization\(^16\) of a generalized-gradient approximation (GGA) to the DFT exchange-correlation functional. The variance in HT-DFT-calculated properties studied in the present work is, therefore, almost entirely due to differences in various parameter choices involved in HT-DFT, and not due to different implementations of DFT or approximations to the exchange-correlation functional.

AFLOW has standardized band structure calculations\(^17\), binary alloy cluster expansions\(^18\), finite-temperature thermodynamic properties\(^19\) calculated for many materials, and has an application programming interface (API) for accessing data\(^20\). The Materials Project includes a variety of properties calculated for specific subsets of materials in the database, including elastic\(^21\), thermoelectric\(^22\), piezoelectric\(^23\), and dielectric\(^24\) properties. It also includes a collection of apps such as a Pourbaix diagram calculator\(^25\), and the underlying data are accessible via an API\(^26\). Finally, the Open Quantum Materials Database (OQMD) contains calculations of a large number of hypothetical compounds based on structural prototypes\(^27–29\), and provides tools for the construction of DFT ground state phase diagrams at ambient and high-pressures\(^30–32\). The OQMD provides the entirety of the underlying database to download all at once, and a RESTful API for programmatic access\(^33\).

We query all three databases for the calculated properties of materials whose crystal structures were sourced from the ICSD and aggregate them onto the Citrination platform\(^34\) after converting records from all sources into a unified, consistent data format, the Physical Information File (PIF)\(^35\). We then generate a set of comparable records for each pairwise combination of the databases—all calculations using the same initial crystal structure, by matching their ICSD Collection Codes (hereafter referred to as “ICSD ID”). In instances where more than one calculation within a single database was labeled with the same ICSD ID, we use the lowest energy calculation for all analysis. In addition, we discard records with obviously unphysical property values, and normalize properties to the same units, where required. We then perform statistical analysis on the final curated set of comparable records across the three databases. Definitions of the metrics used in our analysis are given in Appendix A, and details of the query and curation steps are provided in Section II of the Supplementary Information.

III. RESULTS

The aggregation and processing of the data from the three HT-DFT databases results in a set of \(~70,000\) total comparable DFT calculations. For each property of interest, i.e., formation energy per atom, volume per atom, band gap, total magnetization per formula unit (f.u.), the counts of records, and overlapping records for each pair of databases are shown in Table I. Approximately 15,000–25,000 comparisons can be made for each property and database pair, except for comparisons to formation energies from AFLOW, where only \(~2,200\) records are reported. As mentioned earlier, overlapping records across databases were determined by using exact ICSD ID matches for the reported calculations.

A. Overall pairwise comparison statistics

Table II shows some overall statistics for comparisons of all properties across comparable records in the three
B. Distribution of differences in calculated properties

We first analyze the raw differences in the calculated properties for records overlapping across pairs of databases. Figure 1 shows the distribution of the differences in calculated values for each of formation energy, volume, band gap, and total magnetization, for each pairwise combination of databases.

**Formation energy:** The distribution of differences in calculated formation energy across AFLOW-MP and MP-OQMD is surprisingly bimodal, with peaks around 0 and ±0.2 eV/atom. We find that the peak near 0.2 eV/atom in both pairwise comparisons corresponds mostly to oxides, and a difference in the reference chemical potential of oxygen used to calculate the formation energy. The chemical potential of oxygen in MP is ∼0.4 eV/atom lower than that in AFLOW and OQMD. While the median difference (∆x in Figure 1) are reasonably small across all three pairwise comparisons (up to ∼0.074 eV/atom), the difference distributions for AFLOW-MP and MP-OQMD are rather wide. The median absolute difference (MAD) and the interquartile range (IQR), both robust measures of the spread of a distribution, are up to ∼0.105 eV/atom and ∼0.173 eV/atom, respectively.

**Volume:** The distribution of differences in calculated volumes is skewed towards smaller volumes in the OQMD, but such a skew is absent in the AFLOW-MP comparison. Correspondingly, the median difference between AFLOW and MP volumes are ∼0.01 Å³/atom, whereas the median differences are ∼0.09 Å³/atom for OQMD and ∼0.14 Å³/atom for AFLOW-OQMD and MP-OQMD, respectively. The consistently smaller volumes calculated in the OQMD can be understood to result from the choice of the plane wave energy cutoff used for DFT relaxation calculations. The OQMD chooses a plane wave cutoff that is lower than that used in AFLOW and MP (ENMAX in the POTCAR file, up to 400 eV in OQMD, as opposed to 520 eV in MP and up to 560 eV in AFLOW) for full cell relaxations. The lower plane wave cutoff results in Pulay stresses and generally smaller volumes than fully relaxed calculations. The MAD in volumes for comparisons, especially for OQMD with the other two databases, is up to ∼0.65 Å³/atom.

**Band gap:** The distribution of differences in the calculated band gaps is slightly skewed towards larger band gaps in the OQMD, but this skew is absent in the AFLOW-MP comparison. Correspondingly, the median difference in band gaps between AFLOW and MP is ∼0.01 eV, and up to ∼0.14 eV for comparisons with OQMD. The larger band gaps calculated in the OQMD can be partially understood to also result from the choice of lower plane wave energy cutoffs. Phenomenological theory suggests that a decrease in volume and interatomic distance results in a higher repulsive potential experienced by electrons, resulting in larger band gaps. This
TABLE II. Overall statistics (median absolute difference (MAD), interquartile range (IQR), Pearson’s linear correlation coefficient (r), and Spearman’s rank correlation coefficient (ρ)) for the comparison of properties across HT-DFT databases. For each property, records overlapping across a pair of databases are compared (* for band gap and magnetization, only non-zero values are compared). Generally, lower MAD, lower IQR, higher r, and higher ρ values indicate better reproducibility of calculated properties.

| Property                  | AFLOW-MP | AFLOW-OQMD | MP-OQMD |
|---------------------------|----------|------------|---------|
| Formation Energy (eV/atom)| 0.105    | 0.019      | 0.087   |
| Volume (Å³/atom)          | 0.180    | 0.647      | 0.512   |
| Band Gap (eV)             | 0.078    | 0.209      | 0.178   |
| Total Magnetization (µB/f.u.) | 0.015   | 0.011      | 0.012   |

C. Rank-order comparisons across properties

We next seek to make comparisons across properties. Instead of comparing the raw values of the properties directly, we compare overlapping records using the ordinal rank of the property in each database being compared (hereafter, referred to as “percentile rank”). Comparing the percentile ranks of the properties has a few advantages: (a) It allows for a single consistent metric for comparison across all four properties regardless of the magnitude of the actual value and physical units. (b) It is not affected by many systematic differences, e.g., a constant shift of 0.1 eV in all calculated band gaps in one database. Such constant shifts in calculated properties do not affect the internal consistency of a HT-DFT database, and the percentile ranks which are similarly unaffected capture this property. (c) It is a robust, uniform, identifier of outliers in calculated properties.

Figure 2 consists of percentile rank scatterplots (closely related to the quantile-quantile or Q-Q) plots of each property of interest for each database pair. Note that for band gap (total magnetization), we only include overlapping records where the two databases being compared both report the material to be non-metallic (magnetic), to avoid having to rank near-zero or zero values against one another. A compact line along the diagonal corresponds to perfect correlation between the ranked properties, with more diffuse scattering indicating lower levels of correlation.

Formation energy: Of the four properties, formation energy shows the best correlation between each database pair, consistent with all r and ρ values close to 0.99 in Table II. Nonetheless, there is some off-diagonal scatter for the MP-OQMD comparison for larger (more positive) values of formation energy that is not found in the other database pairs. These calculations correspond to compounds with smaller (positive) formation energies, where the precision necessary to reliably rank the structure approaches the accuracy of the calculation.

Volume: The percentile rank comparison of volume shows higher off-diagonal scatter than that seen in comparisons of formation energy. There is a skew towards higher volumes in AFLOW and MP when compared to OQMD (scatter towards top-left of the diagonal in the AFLOW-OQMD and MP-OQMD comparisons), consistent with the discussion around plane wave energy cutoffs in the previous section.

Band gap: The percentile rank comparison of band
FIG. 1. Distribution of the differences in calculated properties across HT-DFT databases. Each panel corresponds to a property and pair of databases being compared. Solid vertical black lines correspond to the first ($Q_1$) and third ($Q_3$) quartiles of the distribution. The number of records overlapping across the two databases is shown in the top right corner of each panel; the median of distribution ($\tilde{\Delta}x$), the median absolute difference (MAD), and the interquartile range (IQR) are noted on the left.
gap shows even higher off-diagonal scatter than that observed in comparisons of both formation energy and volume. In particular, there is meaningful scatter along the axes, corresponding to cases where one database predicts the material to have a near-zero band gap whereas the other database predicts a (much larger) non-zero band gap.

Total magnetization: The percentile rank comparison of total magnetization per formula unit in all three pairwise comparisons shows a few distinct clusters along the diagonal, corresponding to nominally integer values of magnetic moment per formula unit. There is considerable off-diagonal “bowing” in the comparisons with AFLOW, consistent with the distribution of differences between AFLOW and the other two databases showing a skew towards larger magnetizations in AFLOW and long tails (lower panel in Figure 1). In addition, there is considerable off-diagonal scatter (horizontal and vertical bands in the magnetization panel of Figure 2) indicating significant disagreement between the values reported in the two databases.

Overall, a comparison of rank-ordered properties across two databases shows that formation energies and volumes are more easily reproduced than band gaps and total magnetizations, consistent with correlation coefficients decreasing from ~0.99 for formation energy to ~0.6 for total magnetization (Table II).

D. Reproducibility across materials classes

Intuitively, we expect the level of agreement among the databases to be a strong function of materials class. Therefore, we compare specific subsets of calculations based on various materials classes to elucidate potential causes of differences. The materials classes are defined based on chemical composition, the number of elemental components, the presence of magnetism, band gap, pseudopotential choices, and space group, as summarized in Table III. For classes defined by the output of a calculation (i.e., those based on magnetization and band gap), comparisons are only made if both databases agree that the property has a non-zero value.

Figure 3 contains the median absolute difference relative to the mean (MRAD) values for pairwise comparisons between databases, divided into materials classes as defined in Table III. Cells are colored based on the MRAD value listed. Empty cells correspond to trivial comparisons (e.g., values of band gap where both database agree the structure is metallic). We use MRAD as the metric here to reduce the effect of outliers (as compared to calculating means) as well as to enable comparisons across properties using the same metric. Overall, HT-DFT volumes show the best agreement (lowest MRAD values), from 1–4%. Band gaps show the worst overall agreement (highest MRAD values), 4–10% across all pairwise comparisons. Formation energy comparisons with MP show MRAD values up to 6%, but the AFLOW-OQMD MRAD is only 1.3%. MRAD values for total magnetization vary highly from 0.5% for comparisons with MP to 7.6% for AFLOW-OQMD. In all cases, certain materials classes have distinctly higher or lower MRAD when compared to the MRAD averaged over all materials classes.

Formation Energy: In the comparisons with AFLOW, two materials classes, “Halides” and “Disagree on Metallic”, show the highest MRAD values of up to 14% and 40%, respectively. The high MRAD in halide formation energies can be understood to result from post hoc corrections to the elemental reference energies performed in MP and OQMD, but not in AFLOW, for the halide group of elements (see discussion in Section IV B). The high MRAD of the “Disagree on Metallic” class is likely an artifact of the small formation energies of the few records (~30–50) in the comparison. As noted earlier, since AFLOW reports notably fewer formation energy values than the other databases, the comparisons are made with a much smaller set of records (~2,000). Therefore, we ignore here some of the MRAD outliers in cases where the number of records being compared is very small (e.g., the material class “Magnetic” shows an MRAD of 13% between AFLOW and MP but there are only 5 records in the comparison). Further, the formation energies dataset has very few transition metal, rare-earth, and actinide element-containing compounds (Figures S2 and S6). New, different insights are likely to result from a larger dataset. In the MP-OQMD comparison, with a much larger comparable dataset (~19,000), the “Nitride”, “Pnictide”, and “Chalcogenide” material classes show the highest MRAD values, 14%, 8%, and 11% respectively. This is partly due to differences in fitted elemental chemical potentials for pnictogen and chalcogen elements in MP and OQMD (Section IV B).

Volume: The best agreement is observed in the AFLOW-MP comparisons, with only the “Actinide” material class showing a MRAD greater than 2%. For comparisons with OQMD, the MRAD in volume is generally higher—due to the choice of lower plane wave energy cutoff used for cell relaxation, as discussed earlier (Section III B). The highest MRAD values in the comparisons with OQMD volumes are for the “Nitride” and “Halide” classes (~7–9%). The default plane wave energy cutoffs in the VASP PAW potentials (ENMAX parameter) for N and F are among the highest (400 eV) of all elements. Thus, the lower energy cutoff used by OQMD for relaxation impacts the calculated volumes of nitrides and fluorides the most (Figures S7 and S11). Another material class, “Triclinic”, shows similarly high MRAD values of ~8% in comparisons with OQMD. Upon examination, we find that most triclinic materials in the comparisons are oxides, nitrides, and halides, and thus the high MRAD values are due to the chemical
FIG. 2. Comparison of the calculated properties (formation energy, volume, band gap, and total magnetization) over records overlapping across pairwise combinations of HT-DFT databases plotted as a percentile rank. Overall, formation energies and volumes show better reproducibility than band gaps and magnetizations. The clusters seen in the magnetization comparisons correspond to nominally integer values of magnetic moments.

composition of these compounds rather than their crystal symmetry.

Band gap: While band gap comparisons show the highest MRAD values across properties, some materials classes in particular show MRAD values much greater than \( \sim 10\% \). Of these, in the “Intermetallic” and “Semiconductor” material classes, the MRAD values are expectedly high due to small average band gaps relative to which differences are reported, even though the
Class | Definition
---|---
Oxide | Contains O
Nitride | Contains N
Pnictide | Contains a group 15 element
Chalcogenide | Contains a group 16 element, except O
Halide | Contains a group 17 element
Alkali Metal | Contains a group 1 element, except H
Alkaline Earth Metal | Contains a group 2 element
Transition Metal | Contains a $d$-block element
Metalloid | Contains B, Si, Ge, As, Sb, or Te
Rare-Earth | Contains an element from the lanthanide series
Actinide | Contains an element from the actinide series
Metal-Nometal | Contains at least one metal element and at least one of C, N, O, F, P, S, Cl, Se, Br, I
Intermetallic | Contains only metallic elements
Magnetic | Both databases report a net magnetic moment $> 10^{-2}$ $\mu_\text{B}/\text{f.u.}$
Non-magnetic | Both databases report no net magnetic moment $> 10^{-2}$ $\mu_\text{B}/\text{f.u.}$
Disagree on Magnetic | The two databases disagree on whether a net magnetic moment $> 10^{-2}$ $\mu_\text{B}/\text{f.u.}$ is present
Metallic | Both databases predict a band gap of $< 10^{-2}$ eV
Semiconductor | Both databases predict a band gap between $10^{-2}$ and 1.5 eV
Insulator | Both databases predict a band gap larger than 1.5 eV
Disagree on Metallic | The two databases disagree on whether a band gap $< 10^{-2}$ eV is present
Pseudopotentials Agree | Both databases use the same set of pseudopotentials for all elements
Pseudopotentials Disagree | The databases use different pseudopotentials for at least one element
Elements | Contains only one element
Binaries | Contains two elements
Ternaries | Contains three elements
Quaternaries | Contains four elements
Triclinic | Space group 1–2
Monoclinic | Space group 3–15
Orthorhombic | Space group 16–74
Tetragonal | Space group 75–142
Trigonal | Space group 143–167
Hexagonal | Space group 168–194
Cubic | Space group 195–230

TABLE III. Definitions for the materials classes in used in this work.

absolute differences themselves are not conspicuously large (Figure S1). In other cases, the high MRAD values are a result of (a) different pseudopotential choices for elements (e.g., Cu/Cu_pv, Ce/Ce_3, Eu/Eu_2 choices in the “Disagree on Magnetic” class for the MP-OQMD comparison with an MRAD of $\sim 53$%; see Figure S12), (b) using the GGA or GGA+$U$ approach to calculate properties (e.g., for the “Actinide” material class with MRAD of up to 43% in comparisons with MP), or a combination of both factors (e.g., for the “Metallic” material class with an MRAD of up to 27% in comparisons with AFLOW). Further discussions of these parameter choices are in Section IV.

Total magnetization: While MRAD values in the MP-OQMD comparison are generally small ($< 5$%), some material classes show much higher MRAD values, especially in comparisons with AFLOW. As in the case of band gap values, we find these comparisons to be influenced by pseudopotential choice (of rare-earth elements in particular), GGA+$U$, or both (e.g., the “Metalloid” and “Rare-Earth” material classes in the AFLOW-OQMD comparisons, “Intermetallic” and “Metallic” classes in the AFLOW-MP and AFLOW-OQMD comparisons). We note that some other material classes show high MRAD values, e.g., “Element”, “Binary”, “Ternary”, “Tetragonal”, “Hexagonal”, and “Cubic” (up to MRAD values up to $\sim 50$%) due to, upon further examination, the parameter choices discussed above rather than due to number of components in the compound or crystal symmetry.

Finally, we investigated whether our results hold on a larger comparison set generated by linking very similar ICSD entries by using the crystal structure matching algorithm employed by the Materials Project (see Section II in the Supplementary Information). While some of the quantitative metrics we report varied by a few percent in the expanded comparison, the overall conclusions remain unchanged.
FIG. 3. Median percent absolute differences between properties (formation energy, volume, band gap, total magnetization) calculated in the three databases (AFLOW, MP, OQMD), compared two at a time, across various classes of materials as defined in Table III. The numbers in parentheses indicate the number of overlapping records belonging to the respective material class for a given pair of databases. Trivial comparisons are left blank (e.g., the difference in total magnetization for non-magnetic compounds).

| Property | AFLOW vs MP | AFLOW vs OQMD | MP vs OQMD |
|----------|-------------|---------------|------------|
| All      | 5.8 (60.0)  | 1.3 (38.9)    | 6.3 (29.0) |
| Oxide    | 6.3 (68.9)  | 1.0 (108.4)   | 6.8 (58.1) |
| Nitride  | 4.9 (69.0)  | 4.9 (65.0)    | 4.8 (69.0) |
| Pr nicotine | 6.4 (727)   | 2.4 (570)     | 8.2 (60.5) |
| Chalcogen | 4.2 (108.0) | 1.0 (240.0)   | 10.6 (261.0) |
| Halide   | 14.1 (393)  | 1.7 (281)     | 7.8 (370)  |
| Alkaline Metal | 5.5 (655) | 1.3 (299)    | 6.6 (500)  |
| Alkaline Earth Metal | 4.8 (349) | 0.8 (349) | 5.7 (323) |
| Transition Metal | 4.9 (869) | 1.0 (108.4) | 6.3 (230) |
| Metalloid | 5.7 (680) | 0.8 (20.0) | 5.7 (22) |
| Rare-Earth | 3.0 (1335) | 0.6 (20.0) | 4.8 (1022) |
| Actinide | 9.7 (461) | 4.7 (55) | 6.3 (178) |
| Non-Metallic | 5.8 (1270) | 1.0 (240.0) | 7.4 (44) |
| Disagree On Magnetic | 5.8 (1270) | 1.0 (240.0) | 7.4 (44) |
| Metallic | 2.4 (486) | 1.6 (170) | 3.7 (79) |
| Semiconductor | 4.6 (718) | 0.6 (170) | 7.1 (62) |
| Insulator | 5.0 (1022) | 1.0 (240.0) | 7.1 (62) |
| Pseudopotentials Agree | 5.0 (1022) | 1.0 (240.0) | 7.1 (62) |
| Pseudopotentials Disagree | 5.0 (1022) | 1.0 (240.0) | 7.1 (62) |
| Element | 8.1 (484) | 5.3 (7184) | 9.9 (215) |
| Binary | 8.8 (158) | 5.8 (7184) | 9.9 (215) |
| Ternary | 5.5 (1335) | 1.3 (299) | 5.5 (1335) |
| Quaternary | 5.5 (1335) | 1.3 (299) | 5.5 (1335) |
| Trichloride | 6.0 (1335) | 1.3 (299) | 5.5 (1335) |
| Monochloride | 5.8 (1335) | 1.3 (299) | 5.5 (1335) |
| Orthorhombic | 5.8 (1335) | 1.3 (299) | 5.5 (1335) |
| Tetragonal | 5.8 (1335) | 1.3 (299) | 5.5 (1335) |
| Trigonal | 5.9 (1335) | 1.3 (299) | 5.5 (1335) |
| Hexagonal | 5.7 (1335) | 1.5 (299) | 5.5 (1335) |
| Cubic | 5.7 (1335) | 1.5 (299) | 5.5 (1335) |
IV. DISCUSSION

We discuss some of the most important factors affecting the differences across HT-DFT calculations of properties below. Some of the other factors that either have a minor effect (e.g., post hoc calculation of band gap from band dispersions or density of states) or are specific to a database/property (e.g., plane wave cutoff energy for full cell relaxations in OQMD) have been discussed in the earlier sections.

A. Effects of pseudopotential choice

For nearly all elements, VASP provides multiple PAW potentials to choose from, with different numbers of electrons in the valence. The choice of pseudopotential varies across the HT-DFT databases due to factors such as changes in VASP recommendations and issues of calculation convergence or reproduction of experimental thermochemical data. Interestingly, the choice of pseudopotential has minimal effect on the calculated formation energies and volumes (up to a difference of 1% in cases where pseudopotentials do or do not match; see rows “Pseudopotentials Agree” and “Pseudopotentials Disagree” in Figure 3). On the other hand, the number of valence electrons and consequently the choice of pseudopotential affects the calculated band gaps and magnetization values severely. Especially egregious differences across those properties in material classes such as “Rare-Earth” and “Magnetic” (Figure 3) can be directly traced to different pseudopotential choices. For rare-earth and actinide elements in particular, with \( f \)-electrons that are poorly described by DFT, using pseudopotentials that treat \( f \)-electrons in core or valence can have a significant impact on the calculated band gap (e.g., “Intermetallic” and “Magnetic” classes in Figure 3) and magnetization (e.g., “Rare-Earth” and “Intermetallic” classes in Figure 3) values.

B. Elemental reference states

The largest disagreements in HT-DFT formation energies can be understood to result from different elemental reference states used across databases. To our knowledge, the formation energies reported in AFLOW use DFT total energies of the bulk elements as the reference states, whereas both MP and OQMD use reference energies that are fitted to experimental formation energies. Further, the latter case involves some more choices regarding how the fitted elemental reference states are determined. (a) Should all elemental reference energies be fit to experimental data or only a subset? The OQMD fits only elements whose DFT ground states are poor representation of the experimental reference states (i.e., elements that are gases or that have a solid-solid phase transition below room temperature), whereas MP fits all elemental reference energies. (b) What experimental thermochemical data should be used for fitting, given a lack of a single, widely-accepted set of standard experimental dataset for solids? MP and OQMD use experimental formation energies from different sources to fit elemental reference energies, and this affects calculated formation energies even in cases where the same pseudopotential is used for the element in both databases (e.g., a reference energy of around \(-4.9\) eV and \(-4.5\) eV for O in MP and OQMD respectively). This effect of fitted elemental reference states is shown in the calculated formation energies averaged over compounds containing each element in Figures S2, S6, and S10.

C. GGA vs. GGA+U approach

One of the ways to treat the issue of over-delocalization in DFT is to use the DFT+U approach (or “GGA+U” when used with GGA). Similar to the case of fitting elemental references, using the GGA+U approach requires additional HT-DFT choices. (a) Whether or not to use GGA+U for calculating properties of a given material. All three HT-DFT databases have slightly different sets of compounds for which the GGA+U approach is applied. The OQMD uses GGA+U only for oxides of certain \( 3d \) transition metals (the V–Cu series) and actinide metals. MP uses GGA+U for oxides, fluorides, and sulfides of a larger set of transition metals, but not actinides. AFLOW applies it to an even larger set of compounds, nearly all those containing \( d \)- or \( f \)-block elements. (b) What effective \( U \) value should be used for each element? The three HT-DFT databases all use different effective \( U \) values for each element, obtained either from previous work (OQMD) or in-house parameterization by fitting to experimental data (AFLOW and MP). Further, post hoc corrections are required to maintain consistency between formation energies calculated using the GGA and GGA+U approaches, especially in constructing phase diagrams involving compounds calculated using the two different approaches. Such corrections are obtained by fitting to experimental reaction energies, and can be different between HT-DFT databases based on the source of such reaction energies.

V. CONCLUSION

Recent years have seen a dramatic increase in the application of informatics methods for materials development, using high-throughput DFT data. Several prominent HT-DFT databases exist and each uses different input parameters and post-processing techniques to calculate materials properties. Quantifying the uncertainty in calculated properties due to such parameter choices is therefore crucial to understanding the reproducibility and interoperability of such data. In this work, we centralize data from three of the largest HT-DFT databases,
AFLOW, Materials Project, and OQMD, into a common data platform, allowing records to be accurately compared. We then compare four properties—formation energy, volume, band gap, and total magnetization—of materials calculated in each of the HT-DFT databases using the same initial crystal structure.

Our comparisons show that formation energy and volume are more easily reproduced than band gap and total magnetization. Interestingly, we find that the average difference in calculated properties across two HT-DFT databases is comparable to that between DFT and experiment: up to 0.105 eV/atom for formation energy, 4% for volume, 0.21 eV for band gap, and 0.15 $\mu$B/formula unit for total magnetization. Further, certain input parameter choices disproportionately affect HT-DFT properties of particular classes of materials, e.g. choice of planewave cutoff on formation energies and volumes of oxides and halides, and the choice of pseudopotential on the band gaps and magnetization of rare-earth compounds.

As HT-DFT databases continue to mature, systematic comparisons and standardization of calculations are essential. In particular, we recommend efforts to standardize choices surrounding pseudopotentials, plane wave energy cutoffs, fitting elemental reference energies, using the GGA+$U$ approach, the effective $U$ values used, and post-processing steps to obtain properties such as band gap from the electronic structure.

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DATA AVAILABILITY

All data required to perform the analysis presented in this work are made available via the open Citrination platform (https://citrination.com). The individual datasets can be accessed at https://citrination.com/datasets/187629 (AFLOW), https://citrination.com/datasets/188648 (Materials Project), and https://citrination.com/datasets/187988 (OQMD).
Appendix A: Definitions of statistical quantities

The definitions of statistical quantities and their symbols used in this work throughout are as follows (\(x_i\) and \(y_i\) refer to the two sets of data being compared, e.g. from two different databases):

1. Median difference (\(\tilde{\Delta}x\)):

\[
\tilde{\Delta}x = \text{median}(x_i - y_i)
\]  
(A1)

2. Median absolute difference (MAD):

\[
\text{MAD} = \text{median}(|x_i - y_i|)
\]  
(A2)

3. Interquartile range (IQR):

\[
\text{IQR} = Q_3 - Q_1
\]  
(A3)

where \(Q_1\) and \(Q_3\) are the first and third quartiles (25th and 75th percentiles), respectively.

4. Median relative absolute difference (MRAD):

\[
\text{MRAD} = \text{median}\left(\left|\frac{|x_i - y_i|}{|x_i + y_i|/2}\right| \times 100\right)
\]  
(A4)

5. Pearson correlation coefficient (\(r\)):

\[
r(x,y) = \frac{\sum_i^n (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_i^n (x_i - \bar{x})^2 \sum_i^n (y_i - \bar{y})^2}}
\]  
(A5)

where \(\bar{x} = \frac{1}{n} \sum_i^n x_i\) is the sample mean, and \(n\) is the sample size.

6. Spearman’s rank correlation coefficient (\(\rho\)) is defined as the Pearson correlation coefficient between rank variables \(x^R\) and \(y^R\) corresponding to raw data values \(x_i\) and \(y_i\), respectively:

\[
\rho(x,y) = r(x^R, y^R)
\]  
(A6)

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Supplementary Information for “Reproducibility in high-throughput density functional theory: a comparison of AFLOW, Materials Project, and OQMD”

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I. HT-DFT DATABASES AND MANAGEMENT CODES

Given the popularity of DFT as a method generating materials data, a number of HT-DFT databases with various focus areas have emerged; a list of exemplars is given in Table I. Similarly, codes for the management of these databases, including the workflows to generate the data, have been developed by several groups around the world, such as the packages listed in Table II.

| Database          | Link                                      | Materials                  | Properties                                    | Reference |
|-------------------|-------------------------------------------|----------------------------|-----------------------------------------------|-----------|
| Aflowlib          | materials.duke.edu/aflow.html             | inorganic solids           | electronic structure, thermodynamics          | [1]       |
| Alloy database    | alloy.phys.cmu.edu                        | intermetallics             | structure, cohesive energies                  | [2]       |
| CatApp            | slac.stanford.edu/~strabo/catapp          | molecules on surfaces      | reaction/activation energies                   | [3]       |
| CCCDB             | cccdb.nist.gov                            | atoms, molecules           | thermochemical properties                      | [4]       |
| CMR               | cmr.fysik.dtu.dk                          | perovskites, 2D materials  | energetics, electronic structure              | [5]       |
| CompES-X          | compes-x.nims.go.jp                       | inorganic solids           | electronic structure                          |           |
| Crystalium        | crystalium.materialsvirtuallab.org        | elemental solids           | surface, grain boundary energetics            | [6]       |
| CEP               |                                          | organic photovoltaics      | HOMO-LUMO energies                            | [7]       |
| JARVIS-DFT        | itcns.nist.gov/~knc6/JVASP.html           | 2D/solid inorganics        | elastic, thermoelectric properties            | [8]       |
| NRELMatDB         | materials.nrel.gov                        | inorganic solids           | mechanical, dielectric, piezoelectric         |           |
| Materials Project | materialsproject.org                      | inorganic solids           | quasiparticle energies                         |           |
| NoMaD             | nomad-coe.eu                              | inorganic solids           | raw DFT calculation files                      |           |
| OQMD              | oqmd.org                                  | inorganic solids           | energetics, electronic structure              | [11]      |
| phonondb          | phonondb.mtl.kyoto-u.ac.jp                | inorganic solids           | phonons, thermal properties                   |           |
| TE Design Lab     |                                          | semiconductors             | electronic, thermoelectric properties         | [12]      |

TABLE I. A selection of publicly-available HT-DFT databases.

II. DATA MANAGEMENT

The primary challenge in comparing calculations from different HT-DFT databases is to collect the relevant database entries and determine equivalency between unique calculations of the same structure. This section outlines the workflow of ingesting data from AFLOW, Materials Project, and OQMD into a central repository (the Citrination platform29), all post-extraction processing of the data, the method for querying the post-processed data from Citrination, and the method of determining whether two records were comparable.

A. Importing Data into Citrination

To create a complete and searchable system of records, entries from each HT-DFT database were imported into the Citrination platform29, after standardization into the Physical Information File (PIF) format30 using the pypif31 package. The data in this work represents the data found on the public-facing HT-DFT databases, aggregated in December 2019.

Each HT-DFT database was queried independently using their respective APIs:
TABLE II. A selection of software tools for automating HT-DFT workflows and property calculations.

| Code      | Functionality                                      | Link                                                                 | Reference |
|-----------|----------------------------------------------------|----------------------------------------------------------------------|-----------|
| AiiDA     | calculation setup, submission, storage             | aiida.net                                                           | [14]      |
| ASE       | calculation setup, submission, analysis            | wiki.fysik.dtu.dk/ase                                             | [15]      |
| MPInterfaces | surface calculation setup, analysis                | github.com/henniggroup/MPInterfaces                                | [16]      |
| pymatgen  | calculation setup, analysis                        | pymatgen.org                                                       | [17]      |
| qmpy      | calculation setup, management, analysis            | pypi.org/project/qmpy                                             | [18]      |

Calculation of properties/model building

| Tool       | Description                                      | Link                                                                 | Reference |
|------------|--------------------------------------------------|----------------------------------------------------------------------|-----------|
| Amp        | atomistic potentials                             | amp.readthedocs.io                                                 | [19]      |
| ATAT       | cluster expansions                               | brown.edu/Departments/Engineering/Labs/avdw/atat                    | [20]      |
| atomate    | electronic structure, dielectric tensors         | atomate.org                                                         | [21]      |
| CALYPSO    | crystal structure prediction                      | www.calyposo.cn                                                     | [22]      |
| MAST       | defects, diffusion                               | pythonhosted.org/MAST                                              | [23]      |
| Mint       | crystal structure utilities                       | github.com/materials/mint                                           |           |
| phonopy    | phonons, high-temperature properties             | atztogo.github.io/phonopy                                           | [24]      |
| SeeK-path  | high-symmetry paths in Brillouin zone            | materialscloud.org/work/tools/seekpath                             | [25]      |
| SLUSCHI    | melting temperatures                             | blogs.brown.edu/qhong/?page_id=102                                 | [26]      |
| USPEX      | crystal structure prediction                      | uspex-team.org/en/uspex/overview                                    | [27]      |
| Xtalopt    | crystal structure prediction                      | xtalopt.github.io                                                  | [28]      |

1. AiiDA: The query was performed using the AFLUX API\(^1\), retrieving all records in the icsd catalog. The query resulted in 60,324 records, which were uploaded onto Citrination as PIF objects (https://citrination.com/datasets/187629).

2. Materials Project: The query was performed using the MPRester API\(^{32}\), retrieving all records with non-empty icsd_ids field. The query resulted in 48,833 records, which were uploaded onto Citrination as PIF objects (https://citrination.com/datasets/188648). In addition, some normalized properties such as per-atom volume and per-formula-unit magnetization that were not queried directly but calculated from queried data were added to the PIF objects prior to upload.

3. OQMD: The query was performed using qmpy and a version 1.2 of the underlying database, filtering on FormationEnergy objects associated with converged "static" Calculation objects and Entry objects with "icsd" in the "path" field. The query resulted in 37,989 records, which were uploaded onto Citrination as PIF objects (https://citrination.com/datasets/187988). In addition, some properties that were not directly queried but retrieved as metadata, such as labels of PAW potentials and crystal system, were added to the PIF objects prior to upload.

B. Querying Data from Citrination

The HT-DFT database-specific tags for each of the queried properties are given in Table III. The datasets uploaded onto the Citrination platform can all be queried using a common query language. The common query language enables properties from all three databases to be extracted using the same search key irrespective of the ingested field names. For instance, the number of atoms in the unit cell is extracted as number_of_atoms for all three databases despite varying labels (e.g., nsites, natoms, calculation_output_natoms) across databases.

C. Structure Equivalency

In order to perform a fair comparison between two HT-DFT databases, it is essential to generate a set of equivalent records for each pair of databases considered. We use the ICSD Collection Code(s) (hereafter, “ICSD ID(s)”) in the metadata of each entry to generate a set of comparable records.
TABLE III. HT-DFT database-specific tags for properties compared in this work. In cases where they were not directly queried, normalized values such as per-atom values for “volume” and per-formula unit values for “total magnetization” were calculated from the non-normalized queried data.

1. Exact ICSD ID Matching

The main text contains analysis only for records with the exact same ICSD ID across the two databases being compared at a time, ensuring that the crystal structure of the materials being compared are the same.

2. Aliasing for Multiple ICSD IDs Per Record

Since the former process of exact ICSD ID matching results in a smaller set of records (less than 50%) when compared to the total ICSD entries in each database, we investigated if our results hold on a larger comparison set generated by linking similar ICSD entries. For the process of linking similar ICSD entries, we use the structure comparison and matching algorithm implemented within the Materials Project. The process is involves the following two steps:

STEP 1. Annotation of extracted data with “ICSD UID”

1. Generation of a set of ICSD UIDs from Materials Project: An ICSD UID is defined as a set of ICSD Collection Codes (ICSD IDs) belonging to the same material. Materials Project already groups ICSD IDs per material, but imperfectly. For example, there are three different records for AgO in Materials Project that share the ICSD ID 60625 (https://citrination.com/datasets/187464/show_search?searchMatchOption=fuzzyMatch&systemIdValue=605625). This task in the curation pipeline thus aggregates the ICSD IDs from all three such records to generate a super “ICSD UID”. For instance, GaN (mp-830) was associated with 10 ICSD IDs, and the corresponding ICSD UID is the set of all 10 ICSD IDs: “187047–190412–67781–156260–41546–157511–248504–191770–185155–290614”.

2. Annotation of extracted records with an ICSD UID: First, every record retrieved from Materials Project is matched to an ICSD UID from the set above, depending on the ICSD IDs in the record (the set of ICSD IDs in the record will be a subset of exactly one ICSD UID). Second, it is attempted to match every record retrieved from AFLLOW and OQMD to ICSD UID. If no match is found, the ICSD ID in such a record constitutes a new ICSD UID.

The resulting extracted properties dictionary has the following format:

```json
{
  AFLLOW: [
    {
      db_id: 1,
```
STEP 2. Reverse-mapping properties to ICSD UIDs

This step involves “inverting” the dictionary of extracted properties above such that the ICSD UIDs are the keys and a list of data records corresponding to each UID is the value. The inverted dictionary at this step has the following format:

```
{  
  AFLOW: {  
    icsd_id_1-icsd_id_6-icsd_id_7: [  
      {  
        db_id: 1,  
        prop_name_1: prop_val_1,  
        prop_name_2: prop_val_2,  
      },  
      {  
        db_id: 3,  
        ...  
      }  
    ],  
    icsd_id_2-icsd_id_3: [  
      {  
        db_id: 2,  
        ...  
      }  
    ]  
  },  
  MP: {  
    ...  
  },  
  ...  
}
```
The rest of this document reports data curation performed on datasets generated via “Exact ICSD ID Matching” approach. For the analysis on the larger datasets generated by linking similar ICSD IDs using the structure matching method within MP, a similar curation approach was used.

D. Data Curation

1. Removing composition inconsistencies

From the ICSD UID to properties dictionary above, an ICSD UID key is removed if the entries within it do not have matching compositions. This process is done first within each of the three databases (discarded entries in Table IV), and then for UIDs common to pair-wise combinations of the databases (discarded entries in Table V). Most records filtered out at this step are materials with different number of H and Li atoms (e.g., BaGaH$_4$ vs BaGaH$_5$) or small changes in composition (e.g., Y$_3$Fe$_{29}$ vs Y$_3$Fe$_{31}$).

2. Filtering for the lowest energy entry per ICSD UID

For each ICSD UID, since there may exist multiple entries (calculations) in every database, only the entry with the lowest total_energy_per_atom value is retained from this step onward.

3. Removing records with unphysical properties

At this step, any records with unphysical values of certain properties are removed. This includes all boride formation energies from AFLOW, due to an error in the B chemical potential (this bug was discovered in the course of this work and confirmed by the AFLOW developers$^{33}$). Beyond AFLOW borides, unphysical properties are defined as per-atom formation energies outside $-5$ to $+5$ eV/atom, per-atom volumes above 150 Å$^3$/atom, for all three databases (entries discarded at this step in Table VI).

4. Converting magnetizations into absolute values

Finally, all total_magnetization_per_atom values in all three databases are converted into absolute values.

When querying the Materials Project for total magnetization via the RESTful API, the value returned is not the total magnetic moment of the unit cell, as documented$^{34}$, but rather the per formula unit value. The magnetization values queried from Materials Project were normalized suitably.

Lastly, we identify the largest outliers for each property in each pairwise database comparison post-curation: formation energy in Table VII, volume in Table VIII, band gap in Table IX, and total magnetization in Table X.

| Database | Compositions | ICSD UID |
|----------|--------------|-----------|
| AFLOW    | Bi, YIO, Ba$_2$YCl$_7$, YBrO, Ba$_2$LaCl$_7$, Ba$_2$CeCl$_7$, AgSbTe$_2$ | 0         |
| AFLOW    | LiB, Cr$_2$Te$_3$O$_{11}$ | 1         |
| AFLOW    | BaGaH$_4$, BaGaH$_5$ | 240693    |
| AFLOW    | SrGaH$_4$, SrGaH$_5$ | 240697    |
| OQMD     | ZnCoCuAg, LiMgSnPd | 16478     |

TABLE IV. Instances where composition did not match for records within a database.
TABLE V: Instances where composition did not match for records across two databases being compared.

| Databases         | Compositions                        | ICSD UID |
|-------------------|-------------------------------------|----------|
| AFLOW-MP          | LiZnBi, ZnBi                        | 100115   |
| AFLOW-MP          | Ba₅P₃HO₁₃, Ba₅P₃O₁₃                 | 62283    |
| AFLOW-MP          | RbO₈₂HO₉, RbO₈₂O₉                   | 20611    |
| AFLOW-MP          | Gd₂CBr₂₂, GdBr                      | 47226    |
| AFLOW-MP          | Ba₅Cr₃HO₁₃, Ba₅Cr₃O₁₃               | 21034    |
| AFLOW-MP          | YHO₂, YO₂                           | 28442    |
| AFLOW-MP          | SnPHO₃, SnPO₃                        | 25034    |
| AFLOW-MP          | Na₃VP₂HO₉, Na₃VP₂O₉                 | 50760    |
| AFLOW-MP          | Ta₃Al₄HO₁₄, Ta₃Al₄O₁₄               | 67673    |
| AFLOW-MP          | Y₁₂Fe₃₁, Y₁₂Fe₂₉                   | 107259   |
| AFLOW-MP          | Ga(Bi₂O₇)₃, Ga(Bi₂O₅)₄             | 68646    |
| AFLOW-MP          | NaCHO₂, NaO₂                         | 109643   |
| AFLOW-MP          | KAl₃P₂H₂O₁₁, KAl₃P₂H₄O₁₁            | 407355   |
| AFLOW-MP          | Rb₃H(SO₄)₂₂, Rb₃(SO₄)₂             | 60050    |
| AFLOW-MP          | K₂Cr₂AsHO₁₀, K₂Cr₂AsO₁₀             | 30533    |
| AFLOW-MP          | H₂O, H₂O                             | 27844    |
| AFLOW-MP          | Y₁₂(ReC₃)$_₅$, Y₁₂Re₂C₆             | 658805   |
| AFLOW-MP          | Ba₅Re₃O₁₇, Ba₅Re₃O₁₆                | 100777   |
| AFLOW-MP          | La₃TaH(O₂Cl)₂, La₃Ta(O₂Cl)₃         | 62189    |
| AFLOW-MP          | CdHClO, CdOCl                       | 26752    |
| AFLOW-MP          | Th₃HS₂O₉, Th₃S₂O₉                   | 35358    |
| AFLOW-MP          | NdAl₂, Nd₂Al                        | 608745   |
| AFLOW-MP          | LaNHO₄, LaNO₄                        | 413563   |
| AFLOW-MP          | C₅NH₄₂(O₂F₃)₂, C₅NS₂(O₂F₃)₂         | 50524    |
| AFLOW-MP          | XeSb₂F₁₀, Xe₂Sb₄F₁₉                 | 157666   |
| AFLOW-MP          | HO₃I, O₃I                           | 26621    |
| AFLOW-MP          | NdMoHO₃I₃I₄, NdMoO₃I₄               | 281173   |
| AFLOW-MP          | Dy₂B₂HO₈, Dy₂B₂O₈                   | 413927   |
| AFLOW-MP          | LiCH₂O₃, LiCH₂O₃                    | 109604   |
| AFLOW-MP          | SrHF₃, SrF₃                         | 35408    |
| AFLOW-MP          | Li₂Sc₄P₂HO₈, Li₂Sc₄(PO₄)₂           | 409955   |
| AFLOW-MP          | CaHClO₂, CaOCl                      | 24403    |
| AFLOW-MP          | CaCuAsHO₅, CaCuAsO₅                 | 64694    |
| AFLOW-MP          | BaAl₂HO₈, BaAl₂O₉                   | 33282    |
| AFLOW-MP          | Si₂N₃H, Si₂N₃                      | 202970   |
| AFLOW-MP          | RbHO, Rb₂O₂                        | 61048    |
| AFLOW-MP          | BaHF₃, BaF₃                         | 35409    |
| AFLOW-MP          | HoHO₂, HoO₂                         | 2944     |
| AFLOW-MP          | LiTa₃(Bi₂O₇)₂, Ta₃(Bi₂O₇)₂           | 415141   |
| AFLOW-MP          | Ho₂B₂HO₈, Ho₂B₂O₈                   | 413928   |
| AFLOW-MP          | CdNH₄O₄, CdNO₄                      | 35355    |
| AFLOW-MP          | Na₃TiHF₆, Na₃TiF₈                   | 14131    |
| AFLOW-MP          | HgHO₄Cl, HgO₄Cl                     | 29308    |
| AFLOW-MP          | SrNH₃, SrN                          | 410656   |
| AFLOW-MP          | LaHO₂, LaO₂                         | 60675    |
| AFLOW-MP          | MnP₂HO₇, MnP₂O₇                     | 415152   |
| AFLOW-OQMD        | Y₁₂Fe₃₁, Y₁₂Fe₂₉                   | 107259   |
| AFLOW-OQMD        | Ga(Bi₂O₇)₃, Ga(Bi₂O₅)₄             | 68648    |
| AFLOW-OQMD        | LiB, MnCoSiO₄                       | 2        |
| AFLOW-OQMD        | H₂O, H₂O                            | 27844    |
| MP-OQMD           | Bi₃(PO₅)₂, SmPd                      | 107679   |
| MP-OQMD           | BaGaH₅, BaGaH₄                      | 240893   |
| MP-OQMD           | SrGaH₅, SrGaH₄                      | 240697   |
| Databases       | Composition | $\Delta E_1^f$ (eV/atom) | $\Delta E_2^f$ (eV/atom) | $\Delta E_{1-2}^f$ | ICSD UID |
|-----------------|-------------|--------------------------|--------------------------|---------------------|----------|
| AFLOW-MP        | AlPO$_4$    | −2.780                   | −0.307                   | −2.474              | 162670   |
| AFLOW-MP        | SiO$_2$     | −1.041                   | −2.870                   | 1.820               | 25632    |
| AFLOW-MP        | O           | 0.004                    | 1.669                    | −1.665              | 92775    |
| AFLOW-MP        | AlClO       | −1.741                   | −2.789                   | 1.048               | 27812    |
| AFLOW-MP        | Bi          | 0.135                    | 1.090                    | −0.954              | 51675    |
| AFLOW-MP        | YA$_3$      | 0.515                    | −0.437                   | 0.952               | 58220    |
| AFLOW-MP        | PCl$_5$     | −0.192                   | −1.061                   | 0.869               | 76731    |
| AFLOW-MP        | K$_2$BeO$_2$| −1.259                   | −2.124                   | 0.865               | 23633    |
| AFLOW-MP        | Li$_3$P$_2$O$_7$ | −1.899         | −2.762                   | 0.863               | 39814    |
| AFLOW-MP        | RbC$_8$     | 0.751                    | −0.030                   | 0.781               | 200563   |
| AFLOW-OQMD      | AlPO$_4$    | −2.780                   | −0.237                   | −2.543              | 162670   |
| AFLOW-OQMD      | O           | 0.004                    | 1.395                    | −1.391              | 92775    |
| AFLOW-OQMD      | MgO         | −2.877                   | −1.879                   | −0.998              | 181459   |
| AFLOW-OQMD      | AlClO       | −1.741                   | −2.608                   | 0.867               | 27812    |
| AFLOW-OQMD      | RbC$_8$     | 0.751                    | −0.040                   | 0.791               | 200563   |
| AFLOW-OQMD      | K$_2$BeO$_2$| −1.259                   | −2.002                   | 0.743               | 23633    |
| AFLOW-OQMD      | SrP$_5$Se$_3$| −0.277                | −1.016                   | 0.739               | 412766   |
| AFLOW-OQMD      | Li$_3$P$_2$O$_7$ | −1.899         | −2.634                   | 0.735               | 39814    |
| AFLOW-OQMD      | PCl$_5$     | −0.192                   | −0.908                   | 0.716               | 76731    |
| AFLOW-OQMD      | Mg$_3$P$_2$O$_8$ | −2.346            | −2.930                   | 0.584               | 9849     |
| MP-OQMD         | MnNiAs      | 3.547                    | −0.249                   | 3.796               | 161716   |
| MP-OQMD         | Nd$_3$PbN   | −0.945                   | 1.319                    | −2.264              | 76397    |
| MP-OQMD         | IrC$_4$     | 0.981                    | 3.161                    | −2.180              | 181498   |
| MP-OQMD         | Nd$_3$SnN   | −1.029                   | 1.112                    | −2.214              | 76398    |
| MP-OQMD         | Sm$_3$AlN   | −0.894                   | 1.109                    | −2.003              | 52640    |
| MP-OQMD         | Li$_3$NO$_3$| 0.690                    | −1.252                   | 1.942               | 33661    |
| MP-OQMD         | Pr$_3$AlN   | −0.788                   | 1.101                    | −1.888              | 52639    |
| MP-OQMD         | Cr$_3$O     | 1.971                    | 0.141                    | 1.830               | 15904    |
| MP-OQMD         | Eu(Cu$_2$Sn)$_2$ | 1.296         | −0.322                   | 1.617               | 416796   |
| MP-OQMD         | Gd$_2$Ag    | 1.502                    | −0.102                   | 1.605               | 107733   |

TABLE VI. Records with physically unreasonable values of formation energy (outside the [−5, +5] eV/atom window) and/or volume (>150 Å$^3$/atom).

TABLE VII. Top ten outliers in calculated formation energy across pairwise comparisons of databases.
| Databases       | Composition | $V^1$ (Å³/atom) | $V^2$ (Å³/atom) | $\Delta V$ (Å³/atom) | ICSD UID |
|-----------------|-------------|-----------------|-----------------|---------------------|----------|
| AFLOW-MP        | Bi          | 31.51           | 103.72          | -72.21              | 51675    |
| AFLOW-MP        | MnNiAs      | 15.70           | 84.29           | -68.59              | 161716   |
| AFLOW-MP        | Hg          | 28.86           | 95.21           | -66.35              | 79804    |
| AFLOW-MP        | HoS         | 39.85           | 103.31          | -63.46              | 66357    |
| AFLOW-MP        | SrPSe₃      | 89.79           | 27.94           | 61.85               | 412766   |
| AFLOW-MP        | NbTeBr₃     | 75.01           | 34.92           | 40.09               | 35376    |
| AFLOW-MP        | CeBr₃       | 67.72           | 31.52           | 36.20               | 31582    |
| AFLOW-MP        | Se          | 63.04           | 31.90           | 31.14               | 150731   |
| AFLOW-MP        | FeSeBr₇     | 66.74           | 37.16           | 29.58               | 39528    |
| AFLOW-MP        | SnSe        | 27.09           | 56.42           | -29.34              | 71338    |
| AFLOW-OQMD      | SrPSe₃      | 89.79           | 27.95           | 61.84               | 412766   |
| AFLOW-OQMD      | NbTeBr₃     | 75.01           | 30.71           | 44.30               | 35376    |
| AFLOW-OQMD      | CeBr₃       | 67.72           | 31.01           | 36.71               | 31582    |
| AFLOW-OQMD      | H            | 37.20           | 2.73            | 34.47               | 28465    |
| AFLOW-OQMD      | CsTl        | 14.22           | 47.71           | -33.49              | 165344   |
| AFLOW-OQMD      | Se          | 63.04           | 31.39           | 31.65               | 150731   |
| AFLOW-OQMD      | FeSeBr₇     | 66.74           | 37.22           | 29.52               | 39528    |
| AFLOW-OQMD      | CaPSe₃      | 53.48           | 25.50           | 27.98               | 412765   |
| AFLOW-OQMD      | SnSe        | 27.09           | 52.60           | -25.52              | 71338    |
| AFLOW-OQMD      | TiO₂         | 35.12           | 11.39           | 23.73               | 97008    |
| MP-OQMD         | Bi          | 103.72          | 31.53           | 72.20               | 51675    |
| MP-OQMD         | MnNiAs      | 84.29           | 14.74           | 69.55               | 161716   |
| MP-OQMD         | Hg          | 95.21           | 27.10           | 68.11               | 79804    |
| MP-OQMD         | Co₂O        | 57.55           | 11.71           | 45.84               | 89837    |
| MP-OQMD         | H₂          | 43.46           | 5.38            | 38.08               | 28344    |
| MP-OQMD         | Cd₆Sb₅      | 62.94           | 31.30           | 31.65               | 52833    |
| MP-OQMD         | Cl₂         | 70.98           | 41.47           | 29.50               | 22406    |
| MP-OQMD         | LiBH₄        | 37.31           | 9.87            | 27.44               | 168803   |
| MP-OQMD         | HfPd₃       | 41.53           | 15.69           | 25.84               | 168289   |
| MP-OQMD         | Xe          | 83.51           | 58.86           | 24.65               | 9786     |

TABLE VIII. Top ten outliers in calculated volume across pairwise comparisons of databases.
| Databases     | Composition | $E_{\text{g}}^1$ (eV) | $E_{\text{g}}^2$ (eV) | $\Delta^{1-2}$ (eV) | ICSD UID   |
|---------------|-------------|------------------------|------------------------|----------------------|------------|
| AFLOW-MP      | CeF$_3$     | 5.87                   | 0.00                   | 5.87                 | 42470      |
| AFLOW-MP      | LiAlPHO$_3$ | 0.02                   | 5.72                   | -5.70                | 68921      |
| AFLOW-MP      | Na$_2$PHO$_3$ | 0.00                   | 5.58                   | -5.58                | 155976     |
| AFLOW-MP      | KCeF$_4$    | 5.44                   | 0.00                   | 5.44                 | 23229      |
| AFLOW-MP      | RbYbF$_3$   | 1.09                   | 6.52                   | -5.43                | 49590      |
| AFLOW-MP      | K$_2$NaCe$_2$S$_6$O$_{24}$ | 5.49                 | 0.08                   | 5.41                 | 281576     |
| AFLOW-MP      | CsYbF$_3$   | 1.78                   | 7.05                   | -5.26                | 49579      |
| AFLOW-MP      | BaTm$_2$F$_8$ | 1.97                  | 7.24                   | -5.26                | 20103      |
| AFLOW-MP      | CoPO$_4$    | 5.23                   | 0.00                   | 5.23                 | 184550     |
| AFLOW-MP      | Mg$_3$P$_2$O$_8$ | 0.00                | 5.18                   | -5.18                | 9849       |
| AFLOW-OQMD    | BeF$_2$     | 8.04                   | 0.00                   | 8.04                 | 173557     |
| AFLOW-OQMD    | KYb$_3$F$_{10}$ | 0.97                 | 8.44                   | -7.47                | 28258      |
| AFLOW-OQMD    | NaCaAlF$_6$ | 7.12                   | 0.00                   | 7.12                 | 80542      |
| AFLOW-OQMD    | H$_2$OsCs$_8$N$_2$F$_6$ | 0.00              | 6.68                   | -6.68                | 151185     |
| AFLOW-OQMD    | YbCl$_3$O$_{12}$ | 0.00              | 6.38                   | -6.38                | 85762      |
| AFLOW-OQMD    | LiAlPHO$_3$ | 0.02                   | 6.20                   | -6.18                | 68921      |
| AFLOW-OQMD    | LiEuP$_4$O$_{12}$ | 0.33             | 6.41                   | -6.08                | 416878     |
| AFLOW-OQMD    | Na$_2$PHO$_3$ | 0.00                 | 6.07                   | -6.07                | 155976     |
| AFLOW-OQMD    | CsSiH$_{12}$O$_6$F$_6$ | 0.00          | 5.96                   | -5.96                | 2900       |
| AFLOW-OQMD    | CsYbF$_3$   | 1.78                   | 7.73                   | -5.94                | 49579      |
| MP-OQMD       | KYb$_3$F$_{10}$ | 0.00              | 8.44                   | -8.44                | 28258      |
| MP-OQMD       | BeF$_2$     | 7.96                   | 0.00                   | 7.96                 | 173557     |
| MP-OQMD       | KCeF$_4$    | 0.00                   | 7.75                   | -7.75                | 23229      |
| MP-OQMD       | H$_2$       | 0.00                   | 7.22                   | -7.22                | 28539      |
| MP-OQMD       | NaCaAlF$_6$ | 7.11                   | 0.00                   | 7.11                 | 80542      |
| MP-OQMD       | EuMgF$_4$   | 0.29                   | 7.22                   | -6.94                | 86246      |
| MP-OQMD       | CsEuF$_3$   | 0.00                   | 6.93                   | -6.93                | 49577      |
| MP-OQMD       | H$_2$OsCs$_8$(NF$_3$)$_2$ | 0.17        | 6.68                   | -6.51                | 151185     |
| MP-OQMD       | Yb(CIO$_4$)$_3$ | 0.00             | 6.46                   | -6.46                | 85763      |
| MP-OQMD       | LiEu(PO$_3$)$_4$ | 0.00          | 6.41                   | -6.41                | 416878     |

**TABLE IX.** Top ten outliers in calculated band gap across pairwise comparisons of databases.
| Databases   | Composition | $M^1$ (µB/atom) | $M^2$ (µB/atom) | $\Delta M^{1-2}$ (µB/atom) | ICSD UID |
|-------------|-------------|-----------------|-----------------|---------------------------|----------|
| AFLOW-MP    | YbMn$_{28}$ | 124.89          | 7.16            | 117.72                    | 643923   |
| AFLOW-MP    | Pr$_6$Mn$_{23}$ | 121.85          | 32.42           | 89.43                     | 643337   |
| AFLOW-MP    | BaMn$_{28}$  | 87.51           | 8.61            | 78.90                     | 615966   |
| AFLOW-MP    | Yb$_6$Mn$_{23}$ | 105.23          | 29.18           | 76.05                     | 643920   |
| AFLOW-MP    | Ba$_6$Co$_{25}$S$_{27}$ | 66.99           | 0.00            | 66.99                     | 71939    |
| AFLOW-MP    | Mn$_{20}$W$_3$C$_6$ | 74.10           | 16.64           | 57.46                     | 618279   |
| AFLOW-MP    | Mn$_{20}$Mo$_3$C$_6$ | 73.37           | 16.53           | 56.84                     | 618260   |
| AFLOW-MP    | Gd$_4$Rh$_5$C$_{12}$ | 56.95           | 0.15            | 56.80                     | 617956   |
| AFLOW-MP    | Nd$_{12}$Co$_6$Sn | 56.33           | 0.00            | 56.33                     | 240094   |
| AFLOW-MP    | Yb$_6$Co$_{35}$P$_{19}$ | 56.51           | 1.12            | 55.39                     | 67950    |
| AFLOW-OQMD  | EuMn$_{28}$  | 125.94          | 4.13            | 121.82                    | 631390   |
| AFLOW-OQMD  | Gd$_{13}$Ge$_6$O$_{31}$F | 90.97           | 0.01            | 90.96                     | 62329    |
| AFLOW-OQMD  | Pr$_6$Mn$_{23}$ | 121.85          | 33.03           | 88.82                     | 643337   |
| AFLOW-OQMD  | BaMn$_{28}$  | 87.51           | 5.58            | 82.93                     | 615966   |
| AFLOW-OQMD  | Yb$_6$Mn$_{23}$ | 105.23          | 30.78           | 74.45                     | 643920   |
| AFLOW-OQMD  | Ba$_6$Co$_{25}$S$_{27}$ | 66.99           | 2.23            | 64.76                     | 71939    |
| AFLOW-OQMD  | Nd$_{12}$Co$_6$Sn | 56.33           | 0.01            | 56.32                     | 240094   |
| AFLOW-OQMD  | Gd$_4$Pd$_3$  | 54.76           | 0.89            | 53.86                     | 104112   |
| AFLOW-OQMD  | Gd$_4$Co$_{12}$ | 51.02           | 0.00            | 51.01                     | 245279   |
| AFLOW-OQMD  | ThMn$_{12}$  | 52.10           | 2.25            | 49.86                     | 104986   |
| MP-OQMD     | Gd$_{13}$Ge$_6$O$_{31}$F | 91.00           | 0.01            | 90.99                     | 62329    |
| MP-OQMD     | ZnFe$_{16}$Ni$_7$O$_{32}$ | 38.00           | 94.00           | 56.00                     | 182238   |
| MP-OQMD     | Eu$_7$Au$_3$  | 50.72           | 0.01            | 50.71                     | 611842   |
| MP-OQMD     | Gd$_6$Zn$_{23}$ | 42.88           | 0.01            | 42.87                     | 636504   |
| MP-OQMD     | Gd$_6$C$_3$Cl$_5$ | 42.69           | 0.00            | 42.68                     | 202547   |
| MP-OQMD     | Gd$_{10}$S$_{19}$ | 42.00           | 0.00            | 42.00                     | 416804   |
| MP-OQMD     | Ba$_8$Eu$_3$Cl$_{34}$ | 45.00           | 4.02            | 40.98                     | 408479   |
| MP-OQMD     | Mn$_{18}$Au$_{31}$ | 0.28            | 39.05           | 38.77                     | 58552    |
| MP-OQMD     | Eu$_5$Pd$_2$   | 36.02           | 0.00            | 36.02                     | 631525   |
| MP-OQMD     | Eu$_5$Pt$_2$   | 35.94           | 0.00            | 35.94                     | 631557   |

TABLE X. Top ten outliers in calculated total magnetization across pairwise comparisons of databases.
III. PER-MATERIAL-CLASS MEDIAN ABSOLUTE DIFFERENCES

FIG. S 1. Median absolute differences between properties (formation energy, volume, band gap, total magnetization are in units of eV/atom, Å³/atom, eV, and µB/formula unit, respectively) calculated in the three databases (AFLOW, MP, OQMD), compared pairwise, across various classes of materials as defined in Table III of the main text. The numbers in parentheses indicate the number of overlapping records belonging to the respective material class for a given pair of databases. Trivial comparisons are left blank (e.g., the difference in total magnetization for non-magnetic compounds).

| Property | AFLOW vs MP | AFLOW vs OQMD | MP vs OQMD |
|----------|-------------|---------------|------------|
| All      | (0.195, 0.193, 0.078) | (0.100, 0.091, 0.088) | (0.146, 0.051, 0.002) |
| Oxide    | (0.106, 0.096, 0.048) | (0.101, 0.099, 0.073) | (0.100, 0.092, 0.002) |
| Nitride  | (0.174, 0.217, 0.006) | (0.135, 0.164, 0.002) | (0.132, 0.138, 0.002) |
| Pnicdic  | (0.234, 0.277, 0.004) | (0.230, 0.257, 0.004) | (0.220, 0.243, 0.002) |
| Chalcogenide | (0.135, 0.174, 0.006) | (0.132, 0.169, 0.002) | (0.129, 0.169, 0.001) |
| Halide   | (0.300, 0.307, 0.003) | (0.294, 0.307, 0.003) | (0.291, 0.306, 0.002) |
| Alkali Metal | (0.099, 0.106, 0.004) | (0.099, 0.106, 0.004) | (0.098, 0.099, 0.002) |
| Alkaline Earth Metal | (0.208, 0.209, 0.025) | (0.205, 0.205, 0.025) | (0.204, 0.204, 0.025) |
| Transition Metal | (0.098, 0.108, 0.003) | (0.098, 0.108, 0.003) | (0.097, 0.107, 0.002) |
| Metalloid | (0.156, 0.157, 0.016) | (0.152, 0.152, 0.015) | (0.150, 0.150, 0.015) |
| Rare-Earth | (0.162, 0.162, 0.006) | (0.158, 0.157, 0.006) | (0.156, 0.156, 0.006) |
| Actinide | (0.146, 0.146, 0.031) | (0.145, 0.145, 0.031) | (0.144, 0.144, 0.031) |
| Metal-Nonmetal | (0.128, 0.128, 0.002) | (0.126, 0.126, 0.002) | (0.125, 0.125, 0.002) |
| Intermetallic | (0.099, 0.099, 0.066) | (0.099, 0.099, 0.066) | (0.099, 0.099, 0.066) |
| Magnetic | (0.250, 0.250, 0.002) | (0.248, 0.248, 0.002) | (0.247, 0.247, 0.002) |
| Non-Magnetic | (0.194, 0.194, 0.051) | (0.193, 0.193, 0.051) | (0.192, 0.192, 0.051) |
| Disagree On Magnetic | (0.224, 0.224, 0.033) | (0.222, 0.222, 0.033) | (0.221, 0.221, 0.033) |
| Metallic | (0.007, 0.036, 0.073) | (0.006, 0.035, 0.072) | (0.005, 0.034, 0.071) |
| Semiconductors | (0.032, 0.062, 0.004) | (0.031, 0.061, 0.004) | (0.030, 0.060, 0.003) |
| Insulator | (0.019, 0.018, 0.056) | (0.019, 0.018, 0.056) | (0.018, 0.017, 0.055) |
| Disagree On Insulator | (0.027, 0.027, 0.004) | (0.026, 0.026, 0.004) | (0.025, 0.025, 0.004) |
| Pseudopotentials Agree | (0.115, 0.115, 0.071) | (0.114, 0.114, 0.071) | (0.113, 0.113, 0.071) |
| Pseudopotentials Disagree | (0.063, 0.063, 0.093) | (0.062, 0.062, 0.093) | (0.061, 0.061, 0.093) |
| Element | (0.017, 0.017, 0.042) | (0.016, 0.016, 0.042) | (0.015, 0.015, 0.042) |
| Binary | (0.032, 0.032, 0.048) | (0.031, 0.031, 0.048) | (0.030, 0.030, 0.048) |
| Ternary | (0.133, 0.133, 0.167) | (0.132, 0.132, 0.167) | (0.131, 0.131, 0.167) |
| Quaternary | (0.148, 0.148, 0.098) | (0.147, 0.147, 0.098) | (0.146, 0.146, 0.098) |
| Triclinic | (0.120, 0.120, 0.147) | (0.119, 0.119, 0.147) | (0.118, 0.118, 0.147) |
| Monoclinic | (0.133, 0.133, 0.170) | (0.132, 0.132, 0.170) | (0.131, 0.131, 0.170) |
| Orthorhombic | (0.125, 0.125, 0.125) | (0.124, 0.124, 0.125) | (0.123, 0.123, 0.125) |
| Tetragonal | (0.090, 0.090, 0.190) | (0.089, 0.089, 0.190) | (0.088, 0.088, 0.190) |
| Trigonal | (0.099, 0.099, 0.072) | (0.098, 0.098, 0.072) | (0.098, 0.098, 0.072) |
| Hexagonal | (0.032, 0.032, 0.058) | (0.031, 0.031, 0.058) | (0.030, 0.030, 0.058) |
| Cubic | (0.040, 0.040, 0.093) | (0.039, 0.039, 0.093) | (0.038, 0.038, 0.093) |

FIG. S 1. Median absolute differences between properties (formation energy, volume, band gap, total magnetization are in units of eV/atom, Å³/atom, eV, and µB/formula unit, respectively) calculated in the three databases (AFLOW, MP, OQMD), compared pairwise, across various classes of materials as defined in Table III of the main text. The numbers in parentheses indicate the number of overlapping records belonging to the respective material class for a given pair of databases. Trivial comparisons are left blank (e.g., the difference in total magnetization for non-magnetic compounds).
IV. ELEMENT-WISE ANALYSIS OF HT-DFT DIFFERENCES

To study the source of differences between the various HT-DFT databases, we collect statistics for the four properties being compared—formation energy, volume, band gap, total magnetization—averaged over all records containing a certain element in the periodic table. For each element, we also present the pseudopotential (psp) used in the two databases being compared, and the number of comparable records of compounds containing the element over which statistical quantities are computed.

![AFLOW-MP | Formation energy](image)

**FIG. S2.** Median values of formation energy for compounds containing a certain element in the periodic table, for a comparison of AFLOW and MP. The VASP PAW potential used for each element and the number of records in each comparison are indicated (* indicates more than one pseudopotential used in the database overall for that element).
FIG. S3. Median values of per-atom volume for compounds containing a certain element in the periodic table, for a comparison of AFLOW and MP. The VASP PAW potential used for each element and the number of records in each comparison are indicated (* indicates more than one pseudopotential used in the database overall for that element).

FIG. S4. Median values of band gap for compounds containing a certain element in the periodic table, for a comparison of AFLOW and MP. The VASP PAW potential used for each element and the number of records in each comparison are indicated (* indicates more than one pseudopotential used in the database overall for that element).
FIG. S5. Median values of total magnetization (per formula unit) for compounds containing a certain element in the periodic table, for a comparison of AFLOW and MP. The VASP PAW potential used for each element and the number of records in each comparison are indicated (* indicates more than one pseudopotential used in the database overall for that element).

FIG. S6. Median values of formation energy for compounds containing a certain element in the periodic table, for a comparison of AFLOW and OQMD. The VASP PAW potential used for each element and the number of records in each comparison are indicated (* indicates more than one pseudopotential used in the database overall for that element).
FIG. S7. Median values of per-atom volume for compounds containing a certain element in the periodic table, for a comparison of AFLOW and QMMD. The VASP PAW potential used for each element and the number of records in each comparison are indicated (* indicates more than one pseudopotential used in the database overall for that element).

FIG. S8. Median values of band gap for compounds containing a certain element in the periodic table, for a comparison of AFLOW and QMMD. The VASP PAW potential used for each element and the number of records in each comparison are indicated (* indicates more than one pseudopotential used in the database overall for that element).
FIG. S9. Median values of total magnetization (per formula unit) for compounds containing a certain element in the periodic table, for a comparison of AFLOW and OQMD. The VASP PAW potential used for each element and the number of records in each comparison are indicated (* indicates more than one pseudopotential used in the database overall for that element).

FIG. S10. Median values of formation energy for compounds containing a certain element in the periodic table, for a comparison of MP and OQMD. The VASP PAW potential used for each element and the number of records in each comparison are indicated (* indicates more than one pseudopotential used in the database overall for that element).
FIG. S11. Median values of per-atom volume for compounds containing a certain element in the periodic table, for a comparison of MP and OQMD. The VASP PAW potential used for each element and the number of records in each comparison are indicated (* indicates more than one pseudopotential used in the database overall for that element).

FIG. S12. Median values of band gap for compounds containing a certain element in the periodic table, for a comparison of MP and OQMD. The VASP PAW potential used for each element and the number of records in each comparison are indicated (* indicates more than one pseudopotential used in the database overall for that element).
FIG. S13. Median values of total magnetization (per formula unit) for compounds containing a certain element in the periodic table, for a comparison of MP and OQMD. The VASP PAW potential used for each element and the number of records in each comparison are indicated (* indicates more than one pseudopotential used in the database overall for that element).
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