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Benchmarking the Elastic Tensors of Silicon Polymorphs Across Three Density Functional Theory Databases Disconfirms a Predicted Auxetic Candidate

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Abstract

We benchmark the structural and elastic properties of silicon polymorphs (diamond-Si, BC8-Si, R8-Si, Ibam-Si, and phases identified through high-throughput screening) across three independent computational databases: Materials Project, AFLOW, and JARVIS-DFT. Calibrating against the one phase with a complete experimental elastic tensor (diamond-Si), all three databases show a consistent 9-10% systematic underestimate of the bulk modulus relative to experiment, quantifying a known GGA-PBE limitation across three unrelated codes and workflows. We retrieve and cross-validate the complete elastic tensors of BC8-Si and R8-Si for the first time in a consolidated, source-traceable dataset, confirming both phases mechanically stable and finding BC8-Si to be the most elastically isotropic entry among fifteen independently characterized silicon structures on a symmetry-independent anisotropy index. An apparent auxetic silicon candidate identified by high-throughput screening (derived Poisson ratio -0.181) is shown, via a direct Born-stability-criterion violation in its full elastic tensor, to be mechanically unstable rather than a genuine effect -- illustrating a general pitfall of screening on isotropic averages alone. A component-by-component comparison of the full elastic tensor across eighteen matched AFLOW-JARVIS structures reveals that this agreement is not uniform: two of six diagonal constants, C44 and C66, show median disagreements of 13% and 19% respectively, an order of magnitude larger than the 2-4% typical of normal-stress and off-diagonal constants. This disagreement is absent in cubic structures and present in every non-cubic structure examined; re-pairing C44 against C66 collapses the discrepancy to a few percent in four independent cases, consistent with an axis-labelling convention difference between the two databases rather than a physical one, though genuine structural non-equivalence between matched entries cannot be fully excluded. Mapping the elastic-property space of silicon polymorphs in the style of Ashby materials-selection charts, we find that structural compactness predicts bulk stiffness but has no detectable power to predict ductile-versus-brittle character, a decoupling replicated independently across two of the three databases. We document a genuine, unresolved discrepancy of 11-12% between databases in the bulk modulus of β-Sn-Si, illustrating that cross-database benchmarking remains necessary even for a well-studied elemental system. All underlying data, including full elastic tensors, structure identifiers and evidence-level annotations, are made available in a source-traceable database.

1. Introduction

High-throughput density-functional-theory (DFT) databases -- Materials Project, AFLOW, and JARVIS-DFT among them -- now report computed elastic properties for tens of thousands of inorganic compounds, each generated by an independent code, pseudopotential set, and workflow. Systematic cross-comparison between these databases remains comparatively rare, even though community efforts have repeatedly shown that DFT-computed properties, including elastic constants, carry systematic, method-dependent errors on the order of 10% relative to experiment [15, 16]. Benchmarking is particularly informative for simple, well-characterized elemental systems, where discrepancies cannot be attributed to compositional or structural ambiguity and must instead reflect genuine differences in computational methodology or data curation.

A parallel and increasingly active benchmarking effort targets machine-learned interatomic potentials rather than DFT codes themselves, with platforms such as JARVIS-Leaderboard [23] and CHIPS-FF [24] now providing automated, multi-model comparisons against DFT reference data for exactly this kind of property. That effort is complementary to, rather than a substitute for, the present study: it presumes a trustworthy DFT reference, whereas our focus here is on establishing how much the DFT references themselves already disagree with one another before any machine-learned model is brought into the comparison.

Silicon polymorphs are a natural test case. Diamond-cubic silicon (Si-I) has a complete, well-established experimental elastic tensor, providing a calibration anchor rarely available for more exotic materials. Several metastable high-pressure phases -- BC8-Si (Si-III), R8-Si (Si-XII), and the theoretically predicted Ibam-Si -- have been studied experimentally and computationally for decades, yet their elastic tensors remain incompletely reported in the primary literature. At the same time, high-throughput screening across Materials Project, AFLOW and JARVIS-DFT has independently characterized dozens of additional hypothetical silicon structures, offering a substantial, largely untapped dataset for benchmarking and for materials-selection-style analysis of the elastic-property space silicon polymorphs occupy [20].

This article makes five contributions. First, we consolidate a source-traceable database of silicon-polymorph structural and elastic properties, combining primary literature with targeted queries against three independent high-throughput databases, with every value tagged by its evidence level and provenance. Second, using diamond-Si as a calibration anchor, we quantify the level of agreement between the three databases and experiment. Third, we resolve two specific data-quality anomalies in the screening layer -- a set of mechanically unstable high-symmetry structures and an apparent auxetic candidate -- through direct retrieval and analysis of their complete elastic tensors, rather than relying on derived isotropic averages alone. Fourth, we construct Ashby-style elastic-property maps across the silicon polymorphs in our dataset, showing that structural compactness predicts stiffness but not ductile-versus-brittle character. Fifth, we report a genuine, unresolved three-way discrepancy in the bulk modulus of β-Sn-Si, documented rather than silently averaged away.

2. Database and Methods

2.1 Source-traceable database

The database comprises structural, elastic, electronic and vibrational property records for silicon polymorphs compiled from the primary literature, together with a Materials Project high-throughput screening layer of seventeen additional silicon structures. Every numerical value carries an explicit literature or database reference and an evidence level: DIRECT (reported as-is by a cited source), DERIVED (computed from compatible parameters, e.g. Voigt-Reuss-Hill averages from a reported elastic tensor), DIGITIZED (extracted from a published figure), OPEN (a property not reported anywhere in the audited sources), or CONTEXT (cited for comparative context rather than characterized for that specific phase). No missing datum is artificially completed: hardness and ductility, in particular, are never inferred

from the bulk modulus alone, a practice known to be unreliable across chemically and structurally diverse materials.

2.2 Cross-database query methodology

For structural and elastic properties left incomplete, ambiguous, or internally inconsistent by the primary literature and the Materials Project screening layer, we queried two further independent high-throughput databases directly: AFLOW (via the AFLOW/AFLUX web API) and JARVIS-DFT (via the JARVIS-Tools Python client); Materials Project data were retrieved with the official Materials Project API client (mp-api). All three databases were accessed during September 2026 using the client releases current at that date, and AFLOW queries were issued directly to the AFLUX web endpoint, which carries no client version. Candidate cross-database matches were confirmed by agreement in space group, atom count, and volume per atom, following the same matching logic used internally by these databases' own cross-referencing tools; unconfirmed candidates (for example, a nominal match rejected by inconsistent atom count) were excluded rather than forced. Two data-quality issues were identified and corrected during this process: an inconsistency in the atom-count field returned by one database's summary endpoint across repeated queries for the same entry, resolved by querying the full structure object directly; and a row-duplication artefact in an intermediate consolidation step of one dataset, traced to a non-unique join key and corrected by deduplicating on the database's unique structure identifier. Both corrections are reported in the relevant Results subsections together with their effect on the final dataset.

3. Results

3.1 Calibration against experiment: diamond-Si

Diamond-Si is the only phase in this dataset with a complete experimental elastic tensor (C11 = 165.7, C12 = 63.9, C44 = 79.6 GPa [1]), providing a calibration anchor for the three computational databases. Materials Project (mp-149, GGA-PBE) gives C11 = 153.0, C12 = 57.0, C44 = 74.0 GPa, a systematic underestimate of 7–11% across all three constants (Voigt-Reuss-Hill bulk modulus K_VRH = 89.0 vs 97.8 GPa experimental, -9.0%). An independently compiled AFLOW entry for the same structure (Si2_SG227_cF8, ICSD_150530, AEL/AGL elastic workflow [17]) gives K_VRH = 89.09 GPa, and four matched JARVIS-DFT entries give K = 87.3–88.5 GPa [19]. All three databases agree with each other to within 2% despite using unrelated codes and workflows, and all three confirm essentially the same 9–10% offset from experiment -- a result quantitatively consistent with an independent, 18-material benchmark of GGA-PBE elastic-constant accuracy (~ 10% typical error [15]) and with broader community efforts to systematize DFT error estimation [16].

3.2 Elastic tensors of BC8-Si and R8-Si

The primary literature leaves the elastic tensors of BC8-Si and R8-Si incompletely reported: BC8-Si's primary structural evidence concerns synthesis texture rather than a reported tensor [2], and R8-Si's Rietveld structural refinement does not extend to a full symmetry-specific tensor [3]. Querying Materials

Project directly (mp-168, space group Ia-3; mp-571520, space group R-3; both matched to experimentally observed ICSD structures) retrieves complete tensors for both phases. For BC8-Si (cubic): C11 = 166.0, C12 = 46.0, C44 = 64.0 GPa, giving K = 86.0 GPa, G = 62.4 GPa, and a Zener anisotropy ratio A = 2·C44/(C11-C12) = 1.07 -- within 7% of the isotropic value of 1. For R8-Si (trigonal): C11 = 171.0, C33 = 137.0, C44 = 61.0, C12 = 37.0, C13 = 41.0, C14 = 8.0, C66 = 67.0 GPa, giving K = 79.4 GPa, G = 60.6 GPa. Both tensors satisfy the Born mechanical-stability criteria (all eigenvalues of the 6×6 matrix strictly positive). R8-Si has no counterpart among AFLOW's fifteen validated structures, but an unmatched JARVIS-DFT entry (JVASP-25255) explicitly cross-referenced by JARVIS itself to the same Materials Project identifier gives an independent trigonal tensor (C11 = 174.4, C33 = 140.3, C44 = 69.2, C12 = 36.0, C13 = 36.9, C66 = 62.9 GPa), yielding K = 78.7 GPa and G = 64.3 GPa -- within 0.8% and 6.1% of the Materials Project values respectively, closing what would otherwise be the only one of the four best-characterized phases in this study lacking any independent cross-database validation.

Cross-checking BC8-Si against AFLOW (Si8_SG206_cI16, ICSD_16569) gives K_VRH = 84.68 GPa, within 1.5% of the Materials Project value, but with individual constants (C11 = 171.4, C12 = 41.0, C44 = 63.8 GPa) differing by 3–11% component-by-component -- a reminder that isotropic-average agreement does not guarantee component-level agreement. AFLOW's own Zener anisotropy for this entry is A = 0.979 (just below isotropy) against Materials Project's A = 1.067 (just above it): the two codes disagree on which side of perfect isotropy BC8-Si sits, while agreeing closely on the magnitude of the deviation. A third database, JARVIS-DFT (JVASP-14847/25151), gives K = 81.6 GPa, G = 65.3 GPa, 5% below Materials Project and AFLOW on K but closer to AFLOW on G [19]. A symmetry-independent universal anisotropy index [18] (A^U = 5·Gv/Gr + Kv/Kr-6, zero only for perfect isotropy) places BC8-Si as the single most isotropic entry among all fifteen AFLOW-validated silicon structures in this dataset, against a maximum of 0.72 and a value of 0.24 for ordinary diamond-Si -- a symmetry-independent confirmation that BC8-Si is exceptionally close to elastically isotropic relative to other silicon polymorphs, not an artefact of the cubic-only Zener measure.

3.3 Data-quality patterns in the Materials Project screening layer

Of the seventeen silicon structures in the Materials Project screening layer, two (mp-27, an FCC-Si candidate; mp-1014212, a BCC-Si candidate) show negative derived shear moduli. Direct retrieval of their full tensors confirms genuine mechanical instability rather than a derivation artefact: mp-27 (C11 = 66.0, C12 = 90.0, C44 = 44.0 GPa) violates the Born criterion C11 > C12 (two eigenvalues of the 6×6 matrix equal − 24); mp-1014212 (C11 = 16.0, C12 = 131.0, C44=-10.0 GPa) violates two independent criteria at once, with C44 itself negative. JARVIS-DFT independently flags hypothetical silicon structures in the same space-group families (Fm-3m, Im-3m) as mechanically unstable, with negative shear moduli of its own, though not confirmed to be the identical volume/pressure points. Five further screening-layer structures carry an unconfirmed (VERIFY) rather than locked identification confidence; cross-checking one of them (an entry matched by ICSD number 181908) against both AFLOW and JARVIS-DFT independently gives closely agreeing bulk and shear moduli (AFLOW: 81.4/46.9 GPa; JARVIS: 80.2/46.7

GPa, both within 1.5%), supporting its treatment as a genuine, consistently characterized structure across independent pipelines rather than a database-specific artefact.

3.4 Case study: the mp-2351841 auxetic anomaly

One screening-layer structure, mp-2351841 (dense orthorhombic silicon, space group Cmcm), stands out with a derived Poisson ratio of -0.181, the only negative value among the seventeen structures screened, and a G/B ratio of 2.49 against a range of 0.41–0.76 for the rest of the set. Taken at face value, this suggests auxetic behaviour -- a response very marginally reported for elemental silicon. Systematic prior screening of the entire Materials Project database for homogeneously auxetic compounds identified only three confirmed candidates after DFT verification [14], underscoring how rare a genuine, confirmed auxetic response is among computationally screened inorganic solids and motivating particular scrutiny of an isolated single-structure signal.

Retrieving the complete elastic tensor for mp-2351841 resolves the question directly: C44 = 186.0, C55 = 76.0, C66=-16.0 GPa. A negative diagonal elastic constant violates the Born mechanical-stability criterion outright, meaning mp-2351841 is not a stable structure at all, let alone a genuine auxetic one -- a conclusion corroborated by the structure being flagged theoretical (never observed experimentally) with an energy 0.449 eV/atom above the convex hull, roughly five to ten times the range typically associated with synthesizable metastable phases. The derived negative Poisson ratio is therefore a downstream symptom of mechanical instability, not independent evidence of auxeticity. This case illustrates a general pitfall for high-throughput screening: an isotropic-average-derived Poisson ratio can appear as a striking anomaly while a full-tensor check, straightforward to perform once flagged, resolves it unambiguously and at comparatively low cost. A second, independent example from the JARVIS-DFT screening layer shows the same pitfall in a more severe form: one JARVIS entry (a Cmcm silicon structure unrelated to mp-2351841) carries a nominally unremarkable, small positive derived shear modulus (4.5 GPa), yet its full tensor shows not one but two independently negative diagonal constants (C44=-39.3, C55=-50.1 GPa) -- a case where isotropic averaging very nearly hid a substantially more severe instability than mp-2351841's.

3.5 Elastic-property maps for materials selection

Plotting bulk and shear modulus against structural compactness (volume per atom) in the style of Ashby materials-selection charts [20] provides a compact, practically useful summary of the elastic-property space occupied by silicon polymorphs. Across the fourteen Materials Project screening structures that are neither confirmed artefacts (Section 3.4) nor mechanically unstable (Section 3.3), bulk modulus correlates strongly and significantly with volume per atom (r=-0.75, p = 0.002), and an independently compiled 15-structure AFLOW dataset replicates this relationship closely (r=-0.62, p = 0.014 against volume; r=-0.79, p = 0.0004 against lattice parameter a) -- compactness is, unsurprisingly, a reliable predictor of stiffness.

The same is not true of ductile-versus-brittle character. The Pugh ratio (K/G), the standard elasticity-based ductility indicator, shows no statistically significant correlation with volume per atom in either the Materials Project screening layer ($r = 0.30$, $p = 0.28$) or the independent AFLOW dataset ($r = 0.31$, $p = 0.27$). The clearest illustration is a near-direct contradiction: two of the most compact structures in the Materials Project set (volume per atom differing by less than 6%) fall on opposite sides of the conventional ductile/brittle threshold (K/G = 1.75), one clearly brittle (K/G = 1.35) and the other clearly ductile (K/G = 1.88). For a designer or screening pipeline using density or volume as a quick proxy for elastic behaviour, this is a practically relevant limitation: compactness reliably predicts how stiff a silicon polymorph will be, but not, at this sample size, how it will yield.

This particular contradiction carries a further caveat that reinforces rather than weakens its message. The nominally brittle structure of this pair, identified in Materials Project (space group P6_3/mmc), was independently recomputed by JARVIS-DFT under the same Materials Project cross-reference: JARVIS reports K = 68.98 GPa, G = 11.77 GPa, a Pugh ratio of 5.9 -- extremely ductile, not brittle. The two calculations relax to volumes differing by 11%, and the JARVIS tensor itself violates the exact hexagonal symmetry relation C66=(C11-C12)/2 by 25%, consistent with a numerically delicate calculation near a soft shear mode (C44 and C66 both under 11 GPa, an order of magnitude softer than the normal-stress constants). Rather than undermining the compactness-ductility disconnection reported here, this adds a stronger version of the same point: for at least one structure in this dataset, ductile-versus-brittle classification is not merely uncorrelated with compactness but is itself unstable across independent DFT calculations of the same nominal structure.

3.6 An unresolved discrepancy: β-Sn-Si

Materials Project (mp-92) gives β-Sn-Si a bulk modulus of 107.7 GPa. An independently compiled AFLOW entry with the same space group (I4_1/amd, ICSD_109025) agrees closely (107.8 GPa), though a second AFLOW entry with the same space group (ICSD_41392) gives a shear modulus about 8% lower than the first (55.95 vs 60.66 GPa) -- an internal AFLOW spread between two nominally equivalent ICSD structures. A third database, JARVIS-DFT (three matched entries), disagrees substantially with both: B = 95.4 GPa, roughly 11–12% below the Materials Project and AFLOW values, while its shear modulus (61.4 GPa) sits within the AFLOW spread. This three-way discrepancy in bulk modulus is the largest unresolved cross-database gap found in this benchmark. We report it as an open disagreement between independent high-throughput pipelines for a well-studied elemental phase, rather than adjudicate it without a fourth, independent reference -- illustrating that systematic cross-database benchmarking remains necessary even for simple, well-studied systems.

Table 1
Bulk (K) and shear (G) moduli (GPa) for selected silicon polymorphs across three independent databases and, where available, experiment.

Phase	Property	MP	AFLOW	JARVIS-DFT	Experiment
diamond-Si	K (GPa)	89.0	89.09	87.3–88.5	97.8
BC8-Si	K (GPa)	86.0	84.68	81.6	—
BC8-Si	G (GPa)	62.4	64.32	65.3	—
R8-Si	K (GPa)	79.4	—	—	—
β-Sn-Si	K (GPa)	107.7	107.3-107.8	95.4	—
ICSD_181908 match	K (GPa)	—	81.4	80.2	—

3.7 Which tensor components agree, and which do not

Section 3.2 reported that BC8-Si's isotropic-average bulk modulus agrees between AFLOW and JARVIS-DFT to within 1.5% while individual constants differ by 3–11%. To test whether this pattern generalizes, we compared all 21 independent components of the elastic tensor across the eighteen silicon structures matched between AFLOW and JARVIS-DFT (378 individual component comparisons). Aggregated globally, agreement is excellent (Pearson r = 0.990, MAE = 3.23 GPa, NRMSE = 12.1%), but this aggregate figure masks a sharp, component-specific pattern. The three normal-stress diagonal constants (C11, C22, C33) and most off-diagonal constants (C12, C13, C23) agree closely, with median relative errors of 2.0-3.9% and Pearson correlations of 0.57–0.99 component-by-component. Two of the three shear-diagonal constants, C44 and C66, are markedly less consistent: median relative errors of 13.0% and 19.3% respectively, with weak-to-moderate correlations (r = 0.54 and r = 0.37). The third shear-diagonal constant, C55, agrees as well as the normal-diagonal set (2.1% median relative error, r = 0.78).

A structure-by-structure breakdown (Fig. 6) resolves much of this pattern. The two cubic structures in the matched set, diamond-Si and BC8-Si, show uniformly low disagreement across C44, C55 and C66 alike (0.8–0.9 GPa MAE) -- expected, since cubic symmetry forces C44 = C55=C66 and leaves no room for a labelling ambiguity between them. Every non-cubic structure in the matched set -- hexagonal, tetragonal (two examples) and monoclinic -- shows markedly elevated disagreement concentrated specifically in C44 and C66, ranging from 12.6 to 24.7 GPa MAE. In each of these four cases, re-pairing AFLOW's C44 against JARVIS's C66 (and vice versa) collapses the apparent disagreement to 2–9%, matching the well-behaved components: for example, the monoclinic structure's naive C66 discrepancy (46.8%) becomes 3.7% once compared against JARVIS's C44 instead; the same re-pairing resolves a tetragonal structure's C44/C66 discrepancy (49.3% and 42.8% naive) to 3.0% and 3.8%, and a hexagonal structure's (13.0% and 19.3% naive, in the same direction as the dataset-wide pattern of Fig. 5) to 2.4-3.0%. The monoclinic structure shows the same signature among off-diagonal terms: wherever AFLOW reports a non-zero C14, C24 or C34, JARVIS reports zero there and a matching non-zero C15, C25 or C35 instead, with magnitudes agreeing to 1–8% once re-paired.

This pattern -- disagreement confined to shear-related indices, absent in cubic structures where no labelling choice exists, and resolved by a consistent re-pairing across four unrelated space groups -- is most simply explained by AFLOW and JARVIS-DFT adopting different axis-labelling conventions for non-cubic unit cells (for example, different choices of unique axis in the monoclinic setting), which relabel which Voigt index carries a given physical shear response without changing the underlying physics. We report this as the most likely explanation rather than a confirmed one: the cross-referencing between AFLOW and JARVIS-DFT entries used in this study matches structures by space group, volume per atom and lattice parameters, but has not been verified at the level of atomic positions, so a genuine structural non-equivalence between matched entries -- rather than, or in addition to, an axis convention difference -- cannot be fully excluded. β-Sn-Si (Section 3.6) illustrates that this second possibility is real: its three matched JARVIS entries disagree with each other on individual constants (for example C33 ranges from 123 to 170 GPa across nominally equivalent JARVIS entries), pointing to genuine inter-entry inconsistency rather than a simple, resolvable labelling swap.

A Bland-Altman analysis [21] of the full 378-comparison dataset quantifies this agreement independently of the component-specific breakdown above: the mean bias (AFLOW minus JARVIS-DFT) is 1.60 GPa, with a 95% confidence interval of [0.74, 2.46] GPa that excludes zero -- a small but statistically significant systematic offset, with AFLOW values running slightly higher on average. The 95% limits of agreement are wide, [-15.1, + 18.3] GPa: for any single reported Cij value compared between the two databases, a difference of up to about 15–18 GPa is within normal database-to-database variation, a useful uncertainty bound for anyone using an individual reported constant from either source at face value.

This has a direct practical implication for cross-database benchmarking of elastic properties: agreement on isotropic averages (K, G, E) does not imply agreement at the level of individual tensor components, disagreement is concentrated in specific, identifiable components rather than spread uniformly, and at least part of that disagreement is attributable to bookkeeping conventions rather than physics. Studies that rely on individual Cij values from a single high-throughput database -- particularly C44 or C66 for a non-cubic structure -- would benefit from an explicit component-level cross-check, from testing an axis re-pairing, and from treating any single value as uncertain at the level of the Bland-Altman limits of agreement reported above.

4. Discussion

Read together, this benchmark shows that Materials Project, AFLOW and JARVIS-DFT agree closely -- typically within 1–2% -- on the isotropic elastic averages of well-characterized silicon polymorphs, and all three reproduce the same systematic ~ 9–10% underestimate of the bulk modulus relative to experiment for diamond-Si, consistent with known GGA-PBE limitations. We characterize this specifically as a GGA-PBE functional limitation rather than a generic database limitation, since it is the choice of exchange-correlation functional, not the database infrastructure itself, that is responsible: several of the databases compared here also host, for at least some structures, results computed with meta-GGA (e.g. SCAN, r2SCAN) or hybrid functionals known to reduce this offset, which we did not draw on here because the

screening layer and cross-database matches available for silicon polymorphs were overwhelmingly GGA-PBE; a functional-resolved re-analysis, where higher-fidelity entries exist, is a natural extension of this benchmark rather than a correction to it. This agreement is, however, neither universal nor guaranteed. BC8-Si's individual elastic constants differ by up to 11% between databases despite close agreement in the isotropic average; β-Sn-Si shows an outright unresolved 11–12% discrepancy in bulk modulus, compounded by internal inconsistency among JARVIS-DFT's own matched entries for the same nominal structure; the systematic 378-comparison component analysis of Section 3.7 traces a large fraction of component-level disagreement to a probable axis-labelling convention difference for non-cubic cells, resolved by re-pairing C44 and C66 in four independent cases; and one structure's ductile-versus-brittle classification itself flips between Materials Project and JARVIS-DFT (Section 3.5), the most direct illustration in this study that a single database's classification of a borderline structure should not be taken as definitive. A benchmarking exercise that stopped at isotropic averages from a single database would have missed all four of these findings.

β-Sn-Si's persistent numerical difficulty -- an unresolved three-way discrepancy at the isotropic level (Section 3.6), internal inconsistency among JARVIS-DFT's own matched entries for the same nominal structure, and a severe component-level symmetry violation under AFLOW-JARVIS cross-referencing (Section 3.7) -- is worth situating physically rather than treating as a purely numerical curiosity. Diamond-cubic silicon is theoretically predicted to lose mechanical stability against homogeneous tetragonal shear at a critical pressure of order 64 GPa, with the resulting instability driving a transformation toward the β-Sn structure itself [22]; β-Sn-Si therefore sits, by construction, at the endpoint of a shear-driven structural instability pathway from ordinary silicon. A phase whose defining transformation is a shear instability is a physically plausible candidate for genuinely shear-sensitive, numerically delicate potential-energy-surface curvature under any first-principles method -- consistent with, though not proof of, the pattern observed throughout this benchmark. We note explicitly that our own calculations probe only small-strain linear elastic response at each structure's already-relaxed equilibrium geometry, not the finite-strain transformation pathway itself, so this connection is offered as physical context for why β-Sn-Si is difficult across independent databases, not as a demonstration of the specific mechanism.

The case of mp-2351841 illustrates a related point: screening pipelines that report only derived isotropic quantities (B, G, E, ν from Voigt-Reuss-Hill averaging) can produce striking-looking anomalies -- here, an apparent auxetic response -- that a direct full-tensor check resolves unambiguously and at modest computational cost. We suggest that flagging candidates for full-tensor follow-up specifically when derived quantities are extreme outliers, as done here, is a practical, low-cost complement to whatever stability screening a database already performs internally.

The elastic-property maps of Section 3.5 illustrate a further, more general point of practical relevance for materials selection: structural compactness is a reliable proxy for stiffness in silicon polymorphs but not for ductile-versus-brittle character, a decoupling that held up under independent replication across two unrelated databases despite drawing on largely non-overlapping sets of structures. Interestingly, BC8-Si's elastic isotropy (Section 3.2) contrasts with an independently reported crystallographic texture

developed during its synthesis by indentation [2], a plastic-deformation signature; whether this reflects a genuine decoupling between elastic and plastic anisotropy in this phase is a question this benchmark motivates but does not resolve, since it would require dedicated orientation-resolved mechanical testing beyond the scope of a database comparison.

This work is limited to a single elemental system and to elastic properties; whether the same pattern of cross-database agreement (strong for stiffness, weaker at the component level, occasionally absent altogether for specific phases) generalizes to compound semiconductors or to other property classes remains an open question for future benchmarking work. Our stability assessment throughout is also limited to the Born mechanical-stability criteria applied to the static elastic tensor; we do not compute phonon dispersions or run ab initio molecular dynamics for any structure, so a phase confirmed mechanically stable here could still, in principle, be dynamically unstable (harbouring imaginary phonon modes) or unstable only at finite temperature -- a multi-tier stability assessment combining elastic, phonon and AIMD criteria, standard practice for a definitive stability claim, is not attempted here and would be needed before treating any of the metastable phases discussed as fully validated.

5. Conclusion

Benchmarking the elastic properties of silicon polymorphs across Materials Project, AFLOW and JARVIS-DFT shows close agreement on isotropic averages, calibrated against experiment via diamond-Si to a consistent ~ 9–10% systematic offset, alongside real component-level and phase-specific discrepancies -- most notably an unresolved 11–12% gap in β-Sn-Si's bulk modulus -- that a benchmark relying on a single database would not have revealed. Direct retrieval of full elastic tensors resolves two data-quality anomalies in the screening layer, including an apparent auxetic silicon candidate shown instead to be mechanically unstable, and establishes BC8-Si as the most elastically isotropic structure among fifteen independently characterized silicon polymorphs. Elastic-property maps constructed in the style of Ashby materials-selection charts further show that structural compactness predicts stiffness but not ductile-versus-brittle character in this material system. Beyond silicon, this exercise illustrates the practical value of source-traceable, multi-database benchmarking: agreements build confidence in specific computed values, and disagreements -- reported rather than averaged away -- identify exactly where further calculation or measurement is most needed.

Declarations

Author Contributions

H.A. conceived the study, compiled the database, performed all cross-database queries and analyses reported here, and wrote the manuscript.

Use of Artificial Intelligence

During the preparation of this work, the author used Claude (Anthropic) for generating figures from data the author retrieved directly via the Materials Project, AFLOW and JARVIS-DFT APIs and from the author's own source-traceable database; cross-checking reported literature formulae against their original sources before use; and drafting and editing manuscript text under the author's direction. The author conceived the research questions, executed and interpreted all database queries, directed every analytical choice reported in this work, reviewed and verified all AI-assisted output against the source data, and takes full responsibility for the content, accuracy, and conclusions of this publication.

Conflict of Interest

The author declares no conflict of interest.

Data Availability Statement

The source-traceable database underlying this article, including the primary-literature compilation and the AFLOW and JARVIS-DFT cross-validation datasets, has been deposited in Zenodo under an open license and is citable independently of this article: https://doi.org/10.5281/zenodo.22827377. Materials Project, AFLOW and JARVIS-DFT data are publicly available at their respective repositories and were accessed via their official API clients during September 2026; readers seeking to reproduce a specific query are advised to consult the client versions and access date recorded here.

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Clinical Trial Registration

Not applicable. This study does not involve a clinical trial.

Ethics, Consent to Participate, and Consent to Publish declarations

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Figures

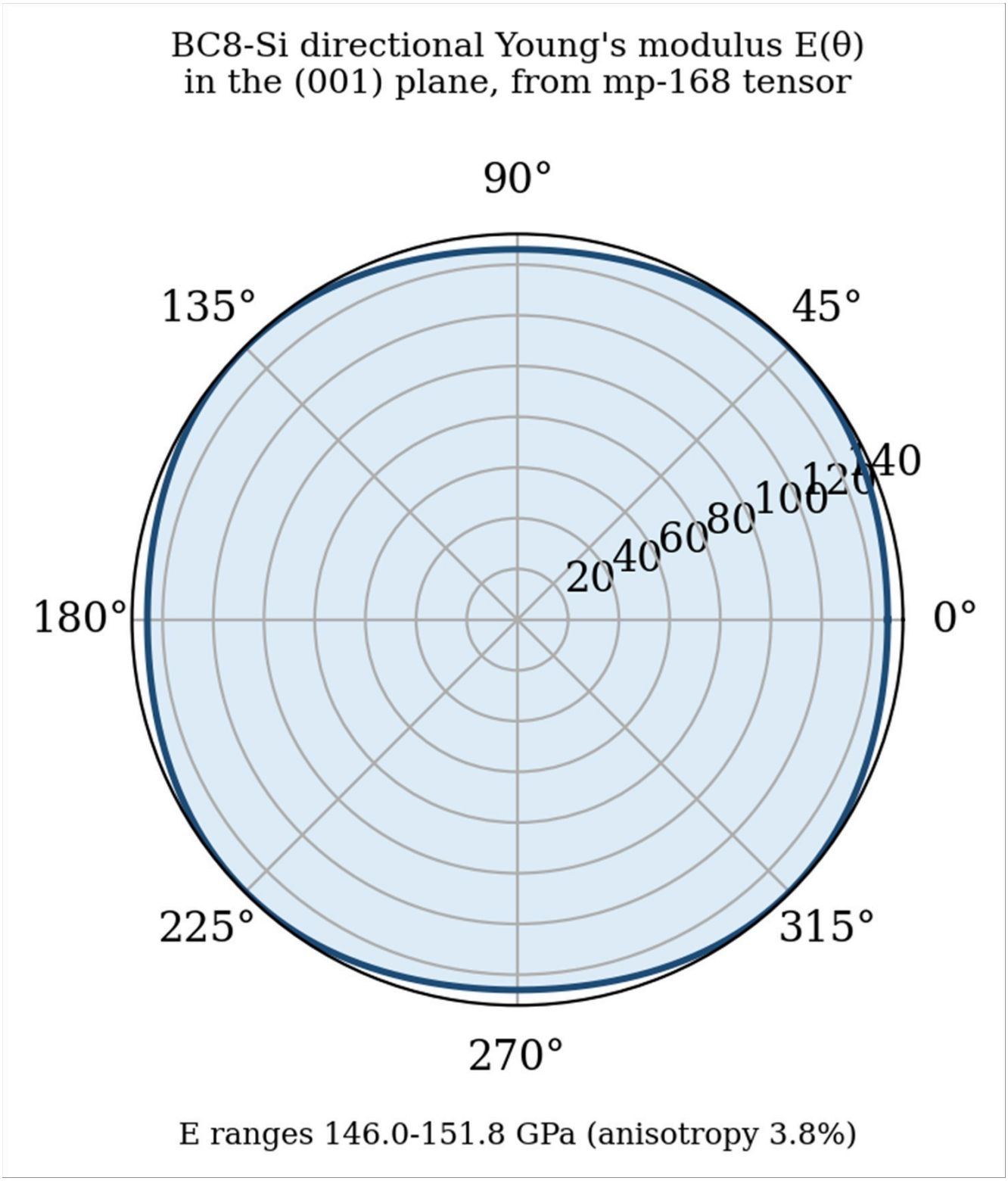


Figure 1

Directional Young's modulus of BC8-Si in the (001) plane, computed from the complete elastic tensor retrieved from Materials Project (mp-168). The near-circular shape (3.8% anisotropy) is a direct, quantitative signature of near-isotropic elastic behaviour.

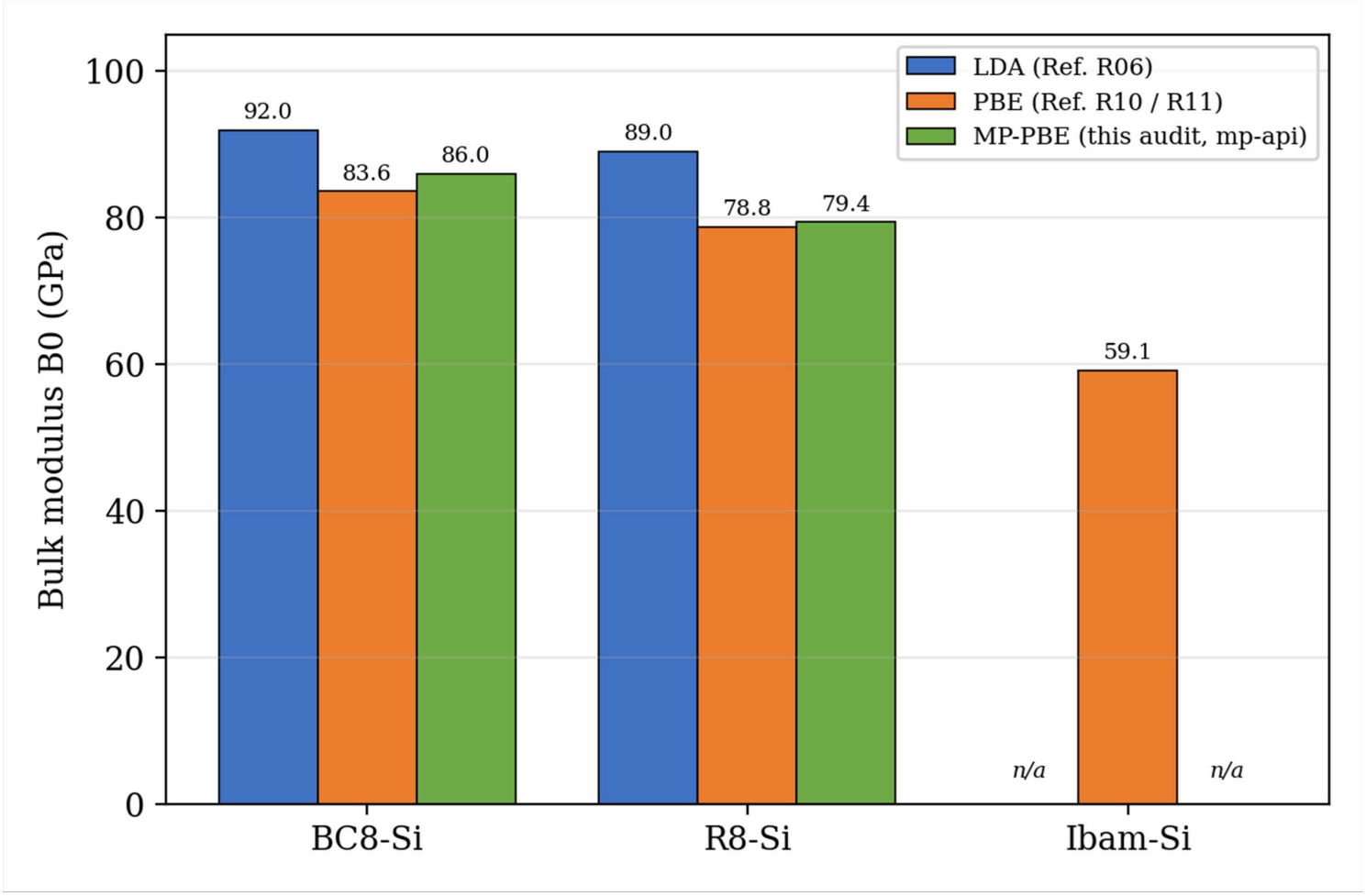


Figure 2

Bulk modulus of diamond-Si, BC8-Si and R8-Si as reported by LDA (Ref. [3]) and PBE (Ref. [6]) literature calculations, and by an independent Materials Project PBE query (this work).

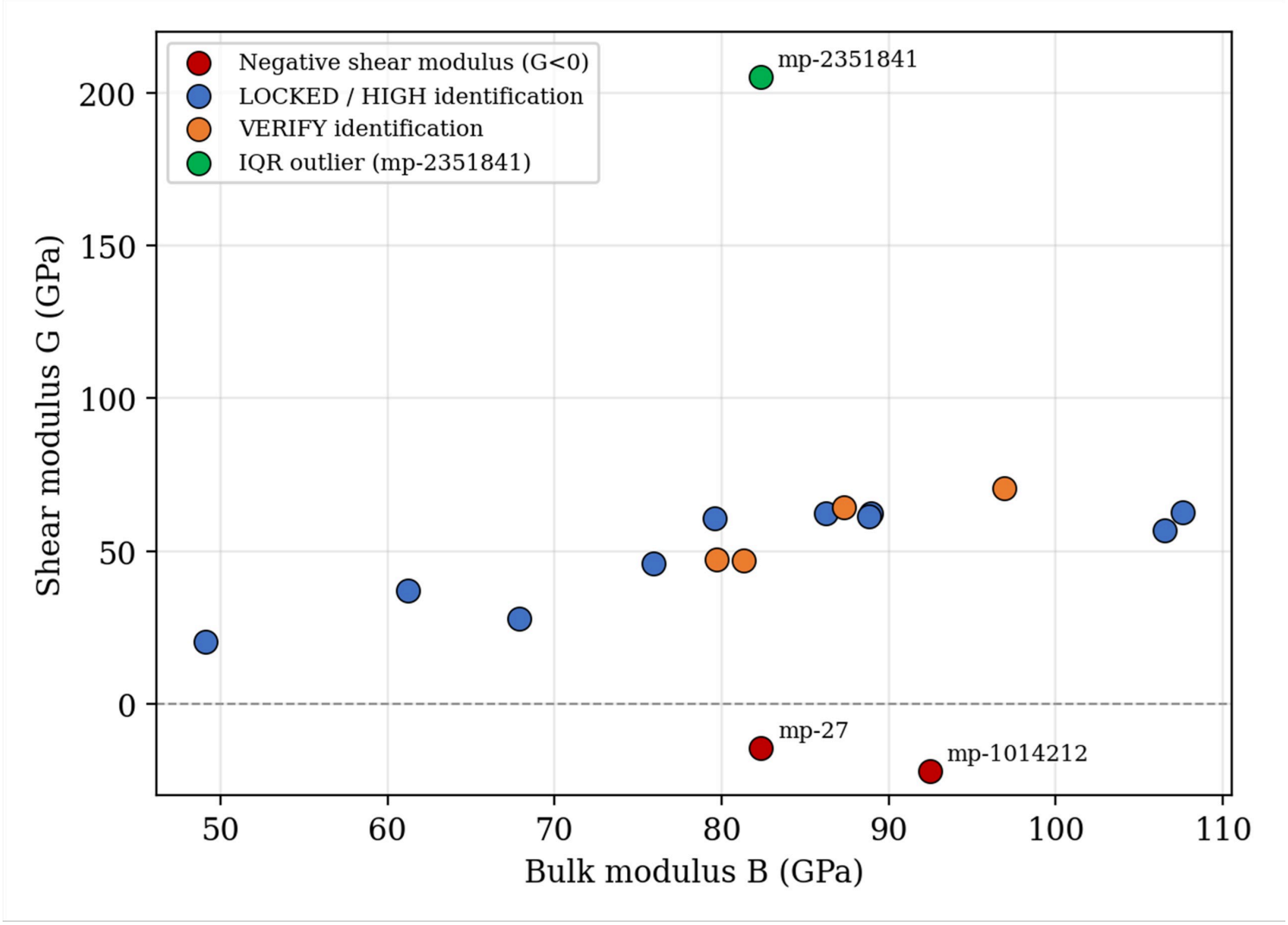


Figure 3

Shear modulus versus bulk modulus (an Ashby-style stiffness map) for the seventeen silicon structures in the Materials Project screening layer. Two structures show non-physical negative G; mp-2351841 (green) is the statistical outlier resolved in Section 3.4.

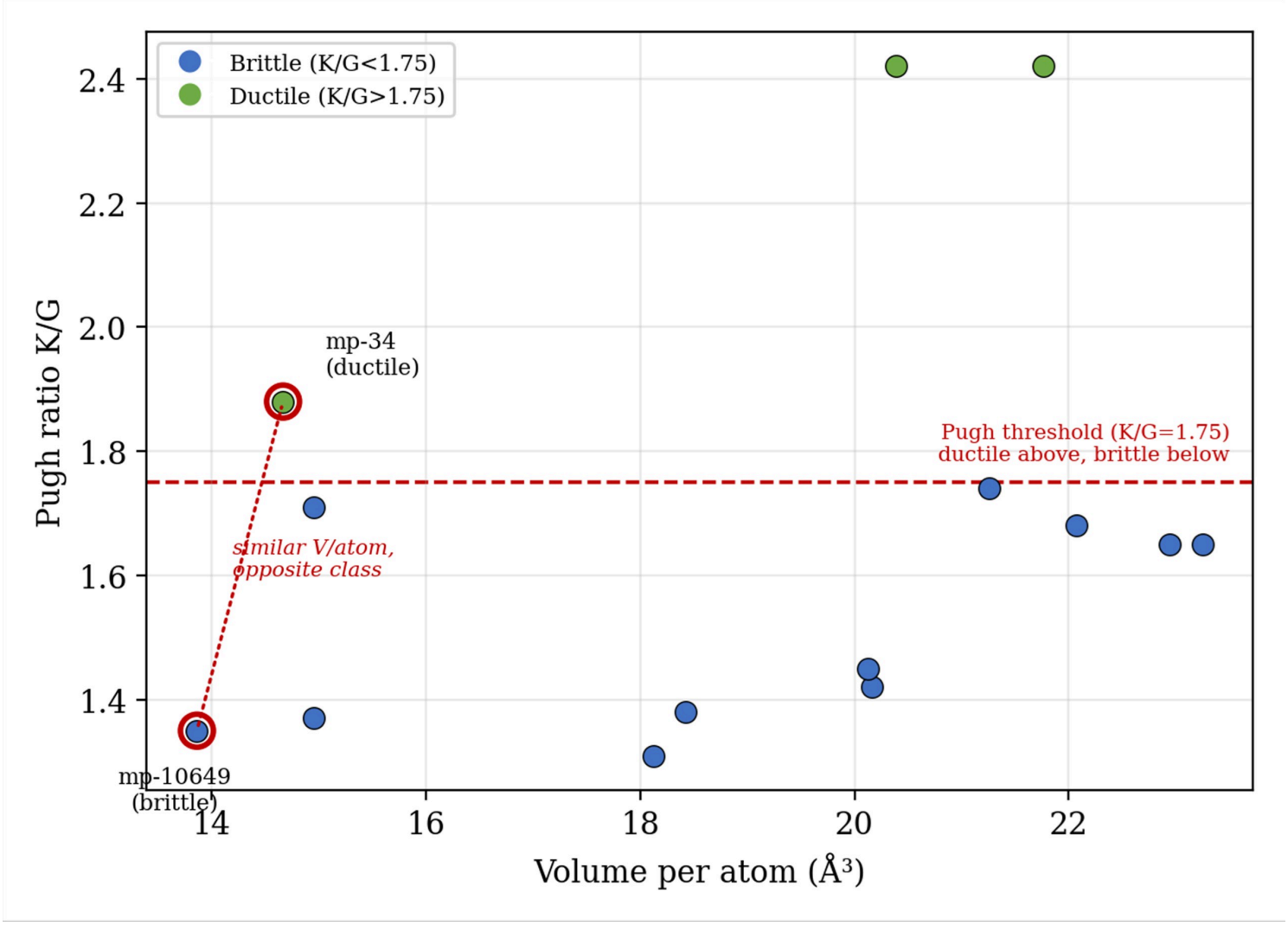


Figure 4

Pugh ratio (K/G, a standard ductility indicator) versus volume per atom -- a materials-selection map showing that, unlike bulk modulus, ductile/brittle character does not correlate with compactness. Two of the most compact structures (circled) fall on opposite sides of the ductile/brittle threshold.

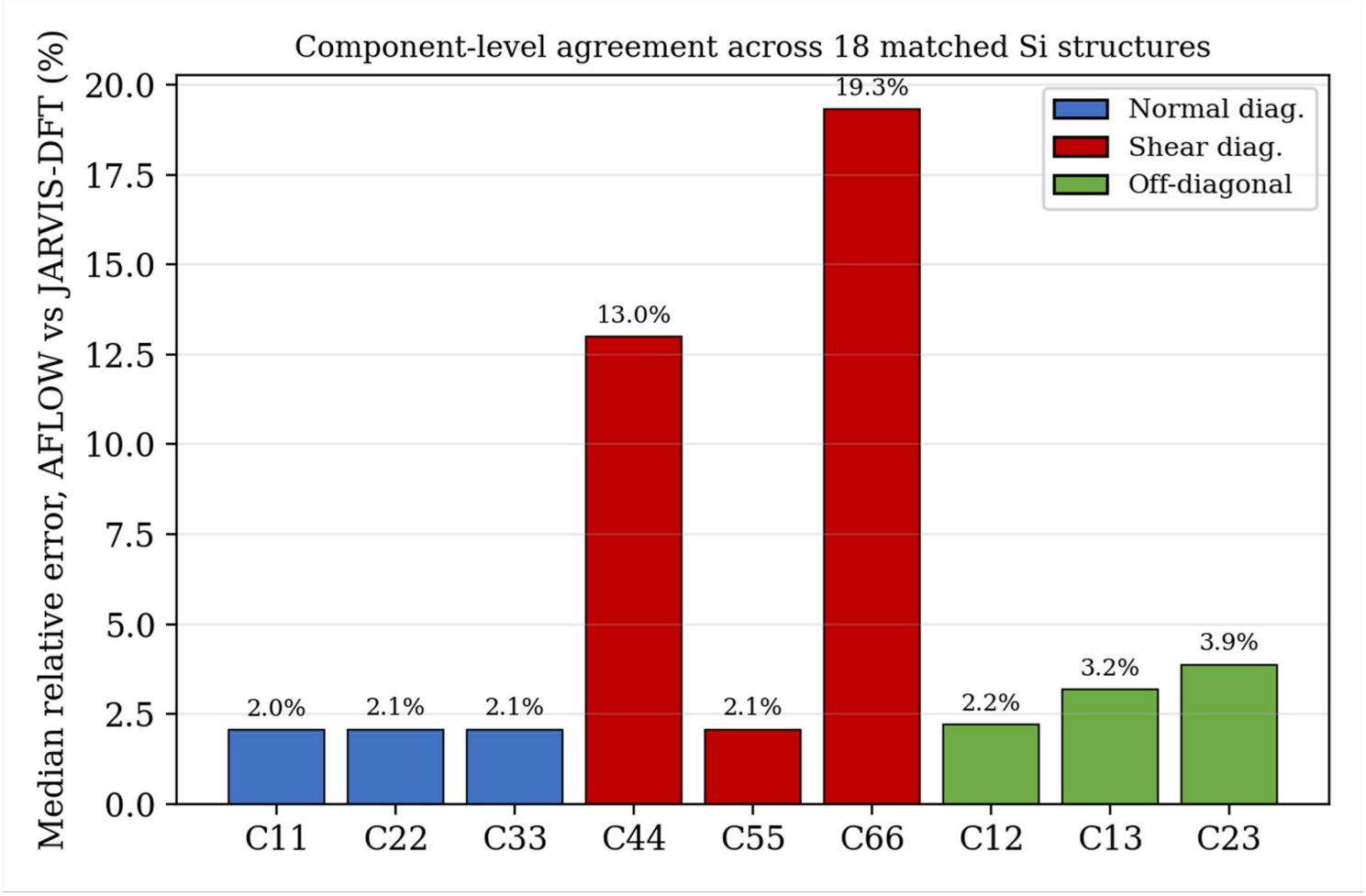


Figure 5

Median relative error between AFLOW and JARVIS-DFT for each independent elastic-tensor component, across 18 matched silicon structures. Normal-stress diagonal and most off-diagonal constants agree to within a few percent; C44 and C66 (shear-diagonal) show 13% and 19% median disagreement respectively, while the third shear-diagonal constant, C55, agrees as well as the normal-diagonal set.

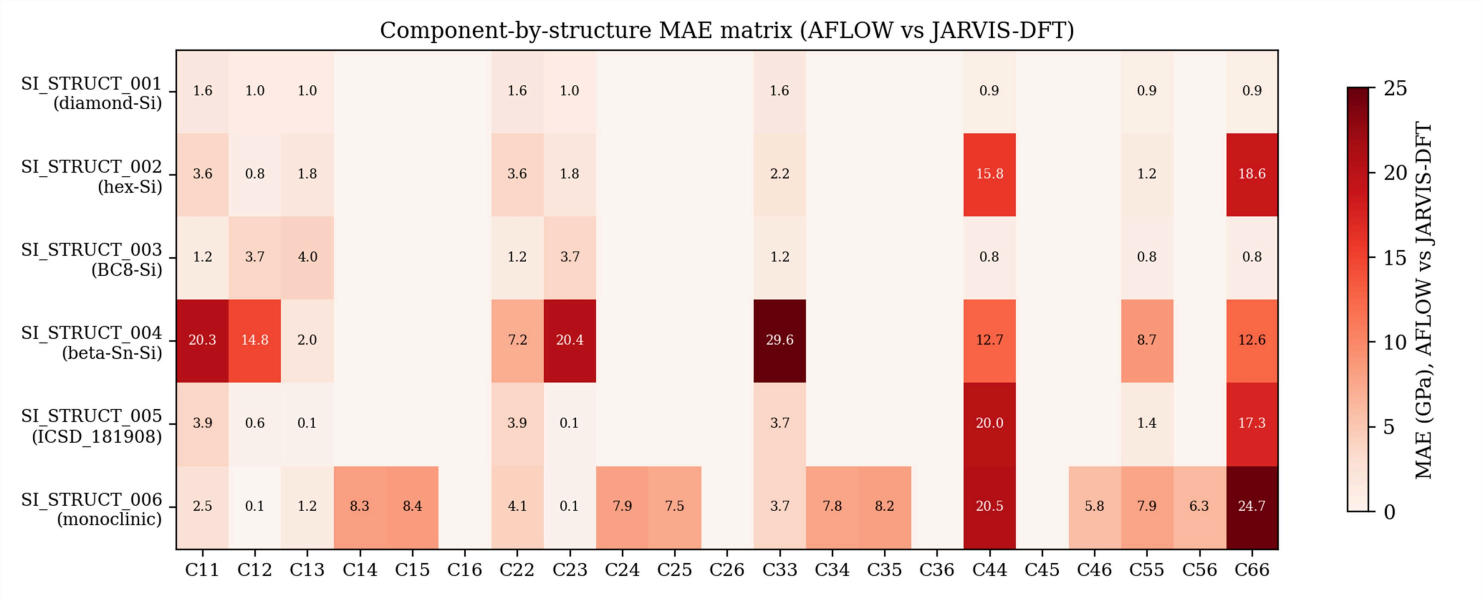


Figure 6

Mean absolute error (GPa) between AFLOW and JARVIS-DFT, broken down by structure and tensor component. The two cubic structures (top two rows) show uniformly low disagreement; every non-cubic structure shows disagreement concentrated in C44 and C66 (and, for the monoclinic structure, in C14/C15, C24/C25, C34/C35), consistent with an axis-labelling difference rather than a physical one.