

Property extraction and limits of verification

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1. Audit of published property extraction

B3.7 continues B3.6 with a property-extraction audit for JVASP-114724. It concerns a retained public record and pinned reference code. Original OUTCAR/vasprun files, the historical calculation procedure and an independent KLT structure remain unavailable. Scientific admission stays BLOCKED.

Observation / check	Result
#11 · DFT-OptB88vdW · original labels	Gap 3.366 eV; CBM 3.652 eV; VBM 7.017 eV. CBM – VBM = –3.365 eV: incompatible with the positive gap.
#11 · separate *_tol fields	CBM 7.017 eV; VBM 3.652 eV. Their difference 3.365 eV is conditionally compatible with 3.366 eV under rounding.
#12 · DFT-TBmBJ	Direct gap 4.638 eV ≥ indirect gap 4.304 eV. Only a necessary ordering relation is checked; no spectrum is reconstructed.
#13 · Voigt bulk	Independent evaluation of the published symmetric tensor gives 163.4 GPa, exactly matching the record.

The 24 September S1 snapshot was restored from the verified B3.6 RESEARCH archive with its SHA-256 unchanged. Retrieval on 26 September returned HTTP 403; the XML is not certified current on that date. Bounded discovery in accessible files found no new original calculation protocols.

Original field names and values are preserved. Internal consistency cannot establish method validity, physical accuracy, convergence or the provenance of a particular run.

2. Reproducing a reference-code label reversal

Three files from the official JARVIS repository were inspected at the same reference revision used in B3.5/B3.6: 2c2241dbd47c7d3ec5f0f7a78e7231e7705b43f7. Retrieved on 26 September, they are hash-pinned and retained in RESEARCH with the original NIST notice [S2-S4].

The non-spin `get_indir_gap` branch computes CBM from the lowest unoccupied level and VBM from the highest occupied level, returning `(gap, cbm, vbm)`. Its spin branch instead assigns the occupied maximum to `cbm` and the unoccupied minimum to `vbm`, while the gap itself retains the correct subtraction [S2]. The serializer writes tuple positions 1 and 2 directly to the CBM and VBM labels [S3].

Synthetic branch	Actual function output
Non-spin-polarized	<code>(gap, CBM, VBM) = (6, 5, -1); CBM - VBM = 6.</code>
Spin-polarized	<code>(gap, CBM, VBM) = (6, -1, 5); CBM - VBM = -6.</code>

Only the extracted AST body of the pinned function was executed on two synthetic NumPy arrays. The JARVIS package was not imported wholesale; no calculation files or VASP process were run. This reproduces a label defect in reference code, not the pilot calculation.

The observed swap is consistent with this mechanism, but its historical cause remains UNVERIFIED. The pilot software revision, ISPIN, NELECT, occupation scheme and eigenvalues are unknown. A published zero magnetic moment does not identify ISPIN. No automatic label correction is applied.

3. Exact compatibility of rounded observations

Theorem (a standard interval result applied to this audit). Let x_i vary independently over nonempty closed intervals $[l_i, u_i]$, and let $y = \sum a_i x_i$. The attainable set of y is exactly $[L, U]$, where:

$$L = \sum \min(a_i l_i, a_i u_i), U = \sum \max(a_i l_i, a_i u_i).$$

Proof. Each linear term reaches its extrema at interval endpoints. Coordinate independence makes all lower extrema and all upper extrema jointly attainable. The linear image of a convex box is convex; in one dimension it fills the interval between its endpoints. Thus a reported interval J is compatible with the model if and only if J intersects $[L, U]$.

If the intervals only enclose correlated quantities, overlap is merely a necessary possibility within the enlarged box model. Narrowing the feasible set cannot repair previously established incompatibility, whereas previous compatibility can disappear. Compatibility does not identify a true value.

$$g = c - v. \text{ For } *_\text{tol}: [L, U] = [3.364, 3.366] \text{ eV}; J = [3.3655, 3.3665] \text{ eV}.$$

A 0.001 eV quantization step gives a closed ± 0.0005 eV enclosure for each field. The intervals overlap although their centers differ by 0.001 eV. With the original labels, $[L, U] = [-3.366, -3.364]$ eV and the intersection is empty.

$$K_V = (C11 + C22 + C33 + 2(C12 + C23 + C31))/9 = 163.4 \text{ GPa}.$$

For $C11=C22=C33=345.0$ and $C12=C23=C31=72.6$ GPa, the displayed values agree exactly. Conditional component errors of ± 0.05 GPa give K_V in $[163.35, 163.45]$ GPa because the absolute coefficients sum to 1. The rounding model follows reference serialization; it is not a physical uncertainty estimate or historical-procedure verification.

4. Quantity types, reproduction and next work

Quantity	Operation supported in this release
Free energy TOTEN	The B3.6 contract remains: explicit energy definition and atom-count normalization.
Band gap, eV	Difference of edges within one method and protocol. No division by the number of atoms.
Bulk modulus K_V, GPa	Linear functional of a bulk tensor in GPa. N/m and asymmetric tensors are rejected; stability is not certified.

Matching units do not establish matching quantity types. OptB88vdW and TBmBJ channels remain separate. TOTEN, energy without entropy and SIGMA→0 extrapolation are not automatically substituted: VASP distinguishes these outputs [S5]. A reported property does not authenticate the energy or normalization of its originating job.

Python 3.11+: `python3 -m unittest discover -s tests -v` runs 28 checks in RESEARCH (20 arithmetic, 8 retained-source checks). `python3 audit_published.py --out my_report.json` reproduces the report offline; output must be new. `python3 reproduce_reference.py` runs two synthetic branches and requires NumPy. PUBLIC runs 20 arithmetic tests; 8 source tests are skipped because the full XML is excluded.

B3.8: obtain primary evidence, independently identify the historical #11 branch, #12 extraction settings and #13 tensor protocol. Until then: science=ABSTAIN; DHC_chem=OPEN-NOT-CONFIRMED; EXT-RUN=NOT_RUN; truth_layer_promotion=0; T6-RA5=NOT_ISSUED; training=CLOSED. All 37 historical blockers remain; none is declared removed. Tomes I-V and earlier publications are unchanged.

S1 · [NIST JARVIS-DFT: JVASP-114724](#); retained 24.09.2026

S2 · [JARVIS Vasprun.get_indir_gap](#), lines 1434-1462

S3 · [JARVIS XML fields and rounding](#)

S4 · [JARVIS ElasticTensor.voigt_modulus](#)

S5 · [VASP Wiki: Smearing technique](#)

S6 · [JARVIS-DFT database documentation](#)