

# Calculation channels and evidence sufficiency

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## 01 / Findings and scope

A working development of Ivan B. Kurpishev’s LOGIC KURPISHEV 2 project: sufficient evidence for ARBD → chemical observation → KLT-MATDES. This release continues B3.3 of 20 September and Site version 23, including later project synchronization. Frozen texts, Tome VI, previous source bytes and scientific statuses are preserved.

| Check                                          | Result                   |
|------------------------------------------------|--------------------------|
| Calculation-channel passports                  | 3: #11, #12, #13         |
| Official index entries                         | 144,895; pilot matches 0 |
| Fresh XML                                      | Matches pinned SHA-256   |
| Authenticated original pilot calculation files | 0 received               |
| New module checks                              | 21 tests passed          |
| Historical blockers                            | 37 retained; 0 removed   |

All 9 groups of the raw\_files index referenced by JARVIS-Tools were checked. This is a 2020 index, not a complete inventory of current storage. Absence of JVASP-114724 is limited to this file. No other material substitutes for the pilot. [S2-S4]

The 24 September XML retrieval matches B3.3 byte for byte. The legacy HTML address returned HTTP 404; download\_files in the pinned XML is empty. Six HTTP attempts retain URL, status and SHA-256; five returned 200. Local retrieval time is not an independent timestamp attestation. [S1]

## Terms have a scope

Figshare metadata assigns CC BY 4.0 to index file 25295732. Its identifier and computed\_md5 match the retrieved file, binding the licence record to this catalogue. Extending it to the OPTIMADE snapshot, XML or pilot calculations is unsupported. The Terms of Use page did not establish applicable permission for our snapshot. [S3-S5]

PUBLIC contains code, synthetic checks, empty evidence templates and audit metadata. Numerical series, property values, coordinates and response bodies remain in RESEARCH.

## 02 / A calculation channel as the audit object

$c = (\text{record\_id}, \text{observation\_id}, \text{method\_class}, \text{xml\_path}, \text{source\_sha256})$ .

The channels differ by method and property extraction: #11 DFT-OptB88vdW; #12 DFT-TBmBJ; #13 DFT-OptB88vdW-Voigt-bulk. Each retains its own B3.3 XML path. Matching a published field does not establish calculation reproducibility.

| Required for each c                              | Current status              |
|--------------------------------------------------|-----------------------------|
| Inputs and software version: INCAR or equivalent | Missing / not channel-bound |
| KPOINTS mesh and construction                    | Missing / not channel-bound |
| Pseudopotential identifiers or digests           | Missing / not channel-bound |
| Outputs: OUTCAR / vasprun or equivalent          | Missing / not channel-bound |
| Extraction of the target property                | Missing / not channel-bound |
| Convergence criterion for this channel           | Unverified                  |

The module accepts a JSON passport and a local evidence directory. It checks record, channel, method, hashes, required roles and path confinement. A complete packet returns `BYTES_COMPLETE_REVIEW_REQUIRED`: technical readiness for content review. Scientific admission remains `BLOCKED`.

Source URLs and file-to-channel bindings in a submission are submitter declarations. Hash matching verifies received bytes against a stated digest. Attribution, file semantics, reviewer independence and computational sufficiency require separate checks.

$\text{admit}(c)$  requires  $B(c) \wedge C(c) \wedge L(c) \wedge K(c) \wedge V(c)$ .

B is byte binding; C verified computational context; L applicable terms; K independent KLT structure mapping; V a separate admission decision. These are necessary conditions, not an implemented admission command. No passport opens training automatically. This evidence-provenance layer does not construct the missing chemical KLT structure.

### 03 / Finite stability and the inference boundary

For strictly increasing settings  $x_1 < \dots < x_N$  and energies  $E_i$ , define the observed suffix radius and diameter. Decimal arithmetic avoids binary-rounding changes to threshold comparisons.

$$r_N(i) = \max_{\{i \leq j \leq N\}} |E_j - E_i|; d_N(i) = \max_{\{j \geq i\}} E_j - \min_{\{j \geq i\}} E_j.$$
$$\text{PASS}(i) \Leftrightarrow N - i + 1 \geq m \text{ and } r_N(i) \leq \epsilon; m = 3, \epsilon = 0.001.$$

The tolerance uses the series units. eV is a general VASP energy convention; run-specific units lack an authenticated primary log. This is an editorial B3.4 diagnostic, not a claim about the provider’s historical criterion.

#### Lemma 1. Unit changes and zero shifts

For  $E'_j = a E_j + b$ ,  $a \neq 0$ , and  $\epsilon' = |a| \epsilon$ ,  $r'_N(i) = |a| r_N(i)$  and  $d'_N(i) = |a| d_N(i)$ ; PASS is invariant. Proof: subtraction cancels  $b$ , absolute values extract  $|a|$ , and the point count is unchanged. This is an exact-arithmetic statement; input rounding can affect boundary cases.

#### Lemma 2. Diameter and radius

$r_N(i) \leq d_N(i) \leq 2r_N(i)$ : the centre  $E_i$  is in the suffix, and the distance between any two values is bounded by the sum of their distances to  $E_i$ . For fixed  $N$  the diameter cannot increase as  $i$  increases, since the set shrinks. No such monotonicity is asserted for the moving-centre radius.

|                                 |                  |
|---------------------------------|------------------|
| Series at its published setting | B3.4 diagnostic  |
| k-parameter: 11 points          | PASS_FINITE_TAIL |
| ENCUT: 6 points                 | FAIL_FINITE_TAIL |

The final point is not evidence of convergence:  $r_N(N)=0$  identically, but  $m=3$  fails. The diagnostic identifies insufficient support under our criterion, not a proven provider error. Neither series is bound to any of the three property channels.

## 04 / Non-identifiability, reproduction and B3.5

### Counterexample: a finite suffix does not determine a limit

Any finite  $E_1, \dots, E_N$  can be continued by  $L, L, \dots$  for an arbitrary  $L$ , yielding limit  $L$ ; another continuation can diverge. Thus a finite-prefix test without an additional model class cannot give a universal limit bound.

Likewise, without an  $E \rightarrow q$  relation, the same total-energy sequence admits formal property outputs  $q_j=0$  and  $q_j=M$  for arbitrary  $M$ . This is a mathematical counterexample to an inference from insufficient premises, not a model of two real substances. Band-gap or elastic-property error bounds require property-specific sequences or a proved error-transfer estimate.

### Meaning for the reper method

In Kurpishev's framework, sufficient reason  $D$  must concern the same observation, method and domain. A source and number define an auditable candidate reper; semantic and physical links remain separate obligations. Philosophically, record stability concerns the evidence, while the truth of a claim about matter needs an additional basis.

### Verification and reproduction

21 tests comprise 18 synthetic and 3 pinned-input integration tests. They cover unit changes, the vacuous last point, arbitrary continuation, channel substitution, altered bytes, path escape, duplicate JSON and status promotion. PUBLIC explicitly skips the three private-input tests. Replaying audit yields identical JSON and requires a new output directory.

B3.5: obtain protocols for #11/#12/#13; explain the ENCUT diagnostic and define each property's criterion; establish terms for pinned data; independently construct and map the KLT structure; reconsider admission by a separate decision. A source-request checklist is prepared; no messages were sent.

science=ABSTAIN; DHC\_chem=OPEN-NOT-CONFIRMED; EXT-RUN=NOT\_RUN; truth\_layer\_promotion=0; T6-RA5=NOT\_ISSUED; axiom\_promotion=DISABLED. Training CLOSED; real forecasts NOT\_RUN; physical\_reachability=NOT\_ESTABLISHED; parameter\_identification=NOT\_PERFORMED.

S1 · NIST JARVIS: JVASP-114724 XML

S2 · JARVIS-Tools: raw\_files catalogue declaration

S3 · Figshare: raw-file index metadata

S4 · Figshare: article metadata API

S5 · JARVIS: Terms of Use