GrantPanel

SAMPLE REPORT · DOE

# GrantPanel DOE Merit Review

## with Recommended Revisions

Merit review under the DOE Office of Science's four criteria (scientific and technical merit, method and approach, personnel and resources, and budget) with three field readers, three rounds of panel discussion, and a consensus recommendation, all generated by GrantPanel's AI review panel.

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PROPOSAL TITLE

### Mechanisms of Ion Transport in Compositionally Disordered Solid Electrolytes

PRINCIPAL INVESTIGATOR

**Dr. Priya Raman**

INSTITUTION

**Northern Plains University**

DOE OFFICE & PROGRAM

**Office of Science · Basic Energy Sciences — Materials Chemistry (Open Call FOA)**

REQUESTED AMOUNT

**$825,000**

DURATION

**36 months**

PANEL CONSENSUS

## Very Good

OVERALL MERIT

The disagreement narrowed but did not fully resolve.

Panel consensus. The proposal advances a testable hypothesis — that compositional disorder in solid electrolytes can be engineered to create percolating low-barrier transport pathways — pursued through a tight loop between quasi-elastic neutron scattering at a DOE user facility and machine-learning-driven molecular dynamics. The panel assessed it against the Office of Science merit criteria in order of importance.

FIX IN THIS ORDER

four of the panel's findings — the full list is below

01 **DMP repository & retention undefined.** →

Name a repository for the neutron-scattering datasets and define retention beyond the award period.

02 **Current & Pending Support incomplete.** →

Add the Co-PI's active LDRD-funded collaboration.

03 **Budget line undocumented.** →

Attach a vendor quote for the year-2 glovebox ($48k).

04 **Basic Research Needs link implicit.** →

Make the connection to BRN priorities explicit.

> This is the short list. The panel filed three independent reviews, argued across three rounds, and produced **five groups of recommended revisions** — including items not shown here. Each finding is tied to the section it came from, so you can check the claim against your own document.

## Contents



## DOCUMENT INTELLIGENCE

### Document Intelligence

Proposal package inventory

READY WITH QUESTIONS

**Detected documents:**

- Project Narrative (pages 1–19)
- Bibliography & References (pages 20–23)
- Budget Justification, Current & Pending Support, and Facilities & Resources are present in the supporting package.

**Conditional requirements:**

- PIER Plan: present. The Promoting Inclusive and Equitable Research plan is included and addresses recruitment and mentoring.
- Letters of collaboration for beamline access: unclear. The Approach depends on synchrotron time, but no facility letter was identified.
- Human subjects and vertebrate animals: not applicable to this work.

**Document quality:** No document quality issues detected.

**Author questions:** Has beamline access been confirmed in writing? Two aims assume scheduled time that the package does not evidence.

## COMPLIANCE & FOA ALIGNMENT

### Compliance

SC FOA formatting & submission check

COMPLETED

**Status:** Compliant with concerns

**Issues found:**

- The Data Management Plan names no repository for the neutron-scattering datasets and does not define retention beyond the award period — SC expects both.
- Current & Pending Support for the Co-PI omits an active LDRD-funded collaboration that appears in the biographical sketch.
- Budget justification: the year-2 equipment line (glovebox, $48k) has no vendor quote attached.

**Notes:** Project narrative is within the page limit (18/20). Biosketches use the required format. Letters of commitment from the SNS beamline scientist and the NERSC allocation request are included.

### FOA Alignment

Does the proposal address the FOA?

COMPLETED

**Alignment:** Strong

**Addressed well:**

- Directly addresses the Materials Chemistry priority on fundamental understanding of ion transport in energy-relevant materials.
- Framing is basic-science throughout — mechanisms, not device engineering — appropriate for an SC program.
- Planned use of DOE user facilities (QENS at the Spallation Neutron Source; NERSC compute) is concrete, with request letters attached.

**Gaps:**

- The FOA asks for an explicit connection to Basic Research Needs priorities; the proposal leaves the mapping implicit.
- The milestone table mixes basic-science outcomes with applied battery metrics in two places (Sec. 6), which a BES panel may read as out of scope.

## INDIVIDUAL MERIT REVIEWS

### Reviewer A
DOE merit reviewer

COMPLETED

RATING — Very Good — OVERALL MERIT

**Summary.** The proposal tests whether tuned cation disorder creates percolating low-barrier pathways in solid electrolytes, combining quasi-elastic neutron scattering with molecular dynamics driven by machine-learned potentials.

**1 · Scientific and/or technical merit**

- The central hypothesis — that disorder can be engineered rather than tolerated — is bold, testable, and could shift how the field approaches superionic conductor design.
- Results would bear directly on the direction of solid-electrolyte research well beyond the specific chemistries studied.
- Novelty relative to the recent high-entropy argyrodite literature is asserted but not fully established (Sec. 2.3).

**2 · Method or approach**

- The QENS–MD feedback loop is sound and the observables are well matched to the simulations.
- Transferability of the machine-learned potential across the composition series needs committed benchmarks.

**3 · Personnel and resources**

- PI has a strong record in neutron spectroscopy of energy materials; facility letters are concrete.

**4 · Budget**

- Generally appropriate; the year-2 equipment purchase deserves scrutiny given institutional resources.

**Overall appraisal.** High scientific merit with a mostly credible approach; supportive of funding.

### Reviewer B
DOE merit reviewer

COMPLETED

RATING — Good — OVERALL MERIT

**Summary.** A QENS-plus-simulation program on disordered solid electrolytes with a machine-learning-potential backbone and a three-composition synthesis plan.

**1 · Scientific and/or technical merit**

- The gap is real, but the influence of the results depends on whether the targeted disorder states can actually be synthesized in a controlled way — under-addressed in Sec. 4.

**2 · Method or approach**

- Central weakness: validation of the machine-learned potentials has no quantitative error targets and no holdout protocol — "agreement with AIMD" is never operationalized.
- No contingency if the SNS beam-time proposal is not awarded; the entire aim-2 timeline assumes first-cycle access.
- Alternative pathways are not discussed; the feasibility logic the criteria ask for is incomplete.

**3 · Personnel and resources**

- Team is competent, but the synthesis effort is understaffed (half a graduate student) for a three-composition matrix.

**4 · Budget**

- Reasonable overall; the glovebox line is not justified against existing institutional equipment.

**Overall appraisal.** Promising science, but the approach needs tightening before full confidence; supportive with reservations.

### Reviewer C
DOE merit reviewer

COMPLETED

RATING — Very Good — OVERALL MERIT

**Summary.** An early-career PI proposes a mechanistic study of disorder-enabled ion transport using DOE user facilities and machine-learned simulations.

**1 · Scientific and/or technical merit**

- Solid and well positioned within the BES portfolio; complements rather than duplicates existing center-scale efforts on solid electrolytes.

**2 · Method or approach**

- Feasible as staged; however, the Data Management Plan does not meet SC expectations — no named repository, no retention commitment for beamline data.

**3 · Personnel and resources**

- Strong early-career trajectory with independent QENS experience — rare and valuable.
- The institution's shared facility already includes a partially available glovebox, which raises questions about the year-2 purchase.

**4 · Budget**

- Year-2 equipment ($48k) overlaps with institutional resources; year-3 travel increase ($9k) is unexplained. A revision of roughly $57k is warranted.

**Overall appraisal.** Fundable with a revised budget and a compliant Data Management Plan.

## PANEL DISCUSSION

### ROUND 1 — POSITIONS

A

**REVIEWER A**

The merit case is the strongest part — engineered disorder is a genuinely new frame. The ML-potential validation gap is real but fixable.

B

**REVIEWER B**

For me the approach is the center of this review: no error targets, no holdout, and no beam-time fallback. Merit doesn't survive an approach that can't deliver it.

C

**REVIEWER C**

Personnel and facilities are strong. My concerns are stewardship-level: the DMP and about $57k of budget need revision — neither is disqualifying.

### ROUND 2 — COUNTER-POINTS

A

**REVIEWER A**

Reviewer B, the PI's prior benchmark study (cited on p.7) partially answers the validation concern — errors under 2 meV/atom on a related chemistry.

B

**REVIEWER B**

Partially conceded — but that was a single composition. Transfer across the disorder series is exactly what's unproven, and the proposal doesn't commit to testing it.

C

**REVIEWER C**

On feasibility: the lab's XRD and impedance capability is a workable fallback if QENS access slips a cycle. The proposal should state that contingency explicitly.

### ROUND 3 — FINAL POSITIONS

A

**REVIEWER A**

Final position: supportive. Merit and personnel carry it; validation plan should be a condition, not a rejection.

B

**REVIEWER B**

Final position: supportive with reservations. I want the validation protocol and beam-time contingency in writing before award.

REVIEWER C

Final position: supportive pending budget revision and a compliant DMP. Recording our disagreement on how severe the validation risk is.

## PANEL RECOMMENDATION

### Panel Summary

Very Good ●●●●○ OVERALL MERIT

**Panel consensus.** The proposal advances a testable hypothesis — that compositional disorder in solid electrolytes can be engineered to create percolating low-barrier transport pathways — pursued through a tight loop between quasi-elastic neutron scattering at a DOE user facility and machine-learning-driven molecular dynamics. The panel assessed it against the Office of Science merit criteria in order of importance.

**1 · Scientific and/or technical merit — consensus**

- Strong. The results would influence the direction and thinking of solid-electrolyte research; after discussion, the panel judged the novelty adequately distinct from the high-entropy literature.

**2 · Method or approach — consensus**

- The QENS–MD–ML loop is credible and the observables are well chosen.
- Consensus weakness: validation of the machine-learned potentials lacks quantitative error targets and a holdout protocol across the composition series.
- A beam-time contingency (lab XRD/impedance pathway) exists but must be stated in the research plan.

**3 · Personnel and resources — consensus**

- Strong early-career PI with independent QENS experience; concrete SNS and NERSC commitments. Synthesis staffing is thin for the proposed matrix.

**4 · Budget — consensus**

- Reasonable in aggregate; the year-2 glovebox ($48k) duplicates institutional resources and the year-3 travel increase ($9k) is unjustified.

**Program policy factors**

- The work fits the Basic Energy Sciences Materials Chemistry mission and does not duplicate efforts currently supported by DOE or other federal agencies, so far as the panel could determine.

**Points of disagreement**

- Severity of the ML-validation risk: Reviewer B considered it an award-gating deficiency; Reviewers A and C viewed it as a condition addressable at award. The disagreement narrowed but did not fully resolve.

**Recommendation.** Recommend for funding contingent on: (1) a quantitative validation protocol for the machine-learned potentials, including holdout compositions; (2) an explicit beam-time contingency plan; (3) a Data Management Plan naming a repository and retention terms; and (4) a budget revision of approximately $57k addressing the equipment and travel items.

## RECOMMENDED REVISIONS

Every weakness and gap the panel raised, paired with a specific, actionable revision, and grouped by review stage.
GrantPanel recommends changes and shows you where; it never edits your document.

### Revisions by section

Ordered by what to fix first

5 REVISIONS

#### 01 Compliance & format

FIX BEFORE SUBMISSION

→ **DMP repository & retention undefined.** Name a repository for the neutron-scattering datasets and define retention beyond the award period.

→ **Current & Pending Support incomplete.** Add the Co-PI's active LDRD-funded collaboration.

→ **Budget line undocumented.** Attach a vendor quote for the year-2 glovebox ($48k).

### 02 FOA alignment

MEET REQUIREMENTS

→ **Basic Research Needs link implicit.** Make the connection to BRN priorities explicit.

→ **Milestone scope drifts to applied metrics.** Remove the applied battery metrics from the milestone table to keep the scope basic-science.

### 03 Individual reviews

STRENGTHEN THE SCIENCE

SCIENTIFIC/TECHNICAL MERIT & APPROACH

→ **ML-potential validation unquantified.** Add quantitative error targets and a holdout protocol across the composition series.

→ **No beam-time contingency.** Add a lab XRD/impedance fallback if SNS access slips a cycle.

→ **Synthesis feasibility under-addressed.** Show the targeted disorder states can be synthesized in a controlled way.

→ **Novelty vs high-entropy work unclear.** Establish distinctiveness from the high-entropy argyrodite literature.

PERSONNEL & BUDGET

→ **Synthesis effort too thin.** Increase effort beyond half a graduate student for the three-composition matrix.

→ **Equipment & travel unjustified.** Justify or remove the glovebox line and the unexplained year-3 travel increase (~$57k revision).

### 04 Panel — priorities

ADDRESS FIRST

→ **Highest priority.** The machine-learned-potential validation protocol (error targets + holdout) and an explicit beam-time contingency.

→ **Then.** A compliant Data Management Plan and the ~$57k budget revision.

### 05 Prior work & citations

POSITION THE CONTRIBUTION

→ **Three directly relevant works under-engaged.** Position against Zeng et al. (Science 2023), and cite the recent MLIP uncertainty-quantification work (2024) and the 2024 QENS study of a related argyrodite series.

## SUPPORTING RESEARCH

### REFERENCES LOOKUP

**References**

Extracts and looks up cited prior work

COMPLETED

Extracting cited references from the proposal...

Found 6 references. Fetching abstracts from Semantic Scholar...

[1/6] Superionic conduction in lithium argyrodites — found [2/6] Foundation models for machine-learned interatomic potentials — found [3/6] Quasi-elastic neutron scattering of lithium diffusion — found [4/6] High-entropy solid electrolytes — found [5/6] FAIR data practices for scattering facilities — no match [6/6] Ab initio molecular dynamics of thiophosphate conductors — found

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The proposal cites 6 references. The abstract or TLDR of each (when available) is provided below to inform your assessment of novelty and prior-work coverage. Cited works without a match in Semantic Scholar are listed by their proposal entry only.

**[1] Superionic conduction in lithium argyrodites** *(2023)* — Ohno et al. *Chemistry of Materials · 2023* We review composition–transport relationships in lithium argyrodite conductors, showing that site disorder between sulfur and halide sublattices correlates strongly with activation energy, and identify open questions about whether disorder can be deliberately controlled during synthesis.

**[2] Foundation models for machine-learned interatomic potentials** *(2024)* — Batatia et al. *arXiv · 2024* We present a large pre-trained interatomic potential covering much of the periodic table and show strong zero-shot accuracy across diverse materials classes, while documenting systematic errors for defect-rich and compositionally disordered systems that fine-tuning only partially removes.

**[3] Quasi-elastic neutron scattering of lithium diffusion** *(2022)* — Mamontov & Sacci *Journal of Physical Chemistry C · 2022* QENS measurements resolve lithium jump rates and residence times in crystalline conductors, providing observables directly comparable to molecular-dynamics correlation functions and establishing the methodology used by subsequent joint experiment–simulation studies.

**[4] High-entropy solid electrolytes** *(2023)* — Zeng et al. *Science · 2023* Configurational disorder in multi-cation lithium conductors flattens the site-energy landscape and raises ionic conductivity by over an order of magnitude, demonstrating entropy engineering as a design axis for solid-state batteries.

**[5] FAIR data practices for scattering facilities** *(Not found on Semantic Scholar.)*

**[6] Ab initio molecular dynamics of thiophosphate conductors** *(2021)* — de Klerk & Wagemaker *Chemistry of Materials · 2021* AIMD simulations of lithium thiophosphates quantify the sensitivity of computed diffusivities to exchange-correlation functional and cell size, cautioning against direct comparison of simulated and measured conductivities without uncertainty analysis.

## LITERATURE REVIEW (DEEP RESEARCH)

### Literature Review

Deep-research SOTA scan

COMPLETED

**Research area & central claim.** The proposal claims that compositional disorder in solid electrolytes can be deliberately engineered to create percolating low-barrier ion-transport pathways, and that a QENS–MD loop with machine-learned potentials can resolve the mechanism. The panel's deep search examined both claims against work from the last three years.

**State of the art (last 2–3 years)**

- Zeng et al. (Science, 2023) established entropy engineering as a conductivity design axis in multi-cation conductors — the closest prior art to the proposal's hypothesis.
- Batatia et al. (2024) released foundation-model interatomic potentials with documented weaknesses on compositionally disordered systems — directly relevant to the proposal's simulation backbone.
- Joint QENS–MD studies (Mamontov and co-workers, 2022–2024) validated jump-diffusion analysis pipelines the proposal adopts.
- Recent argyrodite work (Ohno et al., 2023) mapped disorder–transport correlations but stopped short of controlled disorder synthesis — the gap the proposal targets.
- Uncertainty quantification for MD-derived transport coefficients (de Klerk & Wagemaker, 2021; follow-ups 2024) sets the error-analysis bar the reviewers asked the proposal to meet.

**Competing approaches**

- **High-throughput substitution screening** — broader composition coverage, but without mechanistic resolution of transport pathways.
- **Center-scale battery consortia** — device-oriented; the proposal's basic-science focus is complementary rather than duplicative.
- **Pure-simulation campaigns with foundation potentials** — cheaper, but unvalidated on disordered chemistries; the proposal's experimental loop is its differentiator.

**Open problems the proposal addresses**

- Whether disorder states reachable by synthesis match those that simulations predict to be transport-optimal.
- Quantitative validation of machine-learned potentials across a disorder series — unresolved in the current literature.

**Citation gaps in the proposal**

- Zeng et al., Science 2023 — the closest prior claim to disorder engineering; cited only in passing, not positioned against.
- Recent MLIP uncertainty-quantification work (2024) — directly relevant to the validation protocol reviewers requested; not cited.
- A 2024 QENS study of a related argyrodite series — overlapping observables; not cited.

**Search log**

- "engineered cation disorder solid electrolyte conductivity 2024"
- "high entropy lithium conductor site energy landscape"
- "machine learned interatomic potential disordered materials validation"
- "QENS lithium jump diffusion argyrodite 2024"

- "foundation model interatomic potential fine-tuning error"
- "AIMD conductivity uncertainty quantification solid electrolyte"
- "Spallation Neutron Source QENS energy materials beam time"
- "percolation threshold ion transport disordered crystal"

## INDIVIDUAL WEB SEARCHES

### Reviewer A
3 searches

1. `engineered disorder solid electrolyte novelty 2024`
2. `high entropy argyrodite conductivity mechanism`
3. `QENS MD joint analysis lithium conductor`

### Reviewer B
4 searches

1. `machine learned potential holdout validation materials`
2. `MLIP error target meV/atom benchmark disordered`
3. `SNS beam time award rate general user program`
4. `controlled synthesis cation disorder feasibility`

### Reviewer C
3 searches

1. `DOE SC data management plan repository requirements`
2. `DOE BES early career solid electrolyte portfolio`
3. `university shared facility glovebox budget justification`