View Reviews

Paper ID
186

Paper Title
Quantum-Enhanced Active Learning for Accelerated Materials Discovery

Reviewer #1

Questions

1. Strengths of the Paper
1. The paper addresses an important and timely problem: improving sample efficiency in materials discovery using active learning.
2. Introduces a well-motivated quantum-inspired uncertainty framework that goes beyond classical single-metric uncertainty sampling.
3. The idea of incorporating multi-observable variance and covariance is conceptually strong and well-aligned with the physics of materials systems.
4. The proposed method is model-agnostic and integrates smoothly with standard machine learning models such as random forests and neural networks.
5. Extensive experimental validation is provided on two representative materials science tasks with:
- Multiple strong baselines,
- Multiple random seeds,
- Statistical significance testing.
6. The paper demonstrates clear empirical benefits, including faster convergence and reduced experimental budget.
7. The work emphasizes reproducibility, with code and preprocessing scripts publicly released.
8. The manuscript is well-structured, clearly written, and easy to follow

2. Shortcomings in the Paper

1. The quantum observables are hand-designed, which may limit generalization and scalability to other domains or properties.
2. The multi-observable uncertainty is ultimately reduced to a single scalar acquisition score, potentially discarding richer trade-offs between objectives.
3. Evaluation is limited to two regression tasks; no classification tasks or real experimental (wet-lab or autonomous lab) validation is included.
4. The approach is quantum-inspired only; no comparison with actual quantum hardware or quantum simulators is provided.
5. Computational complexity is discussed theoretically, but runtime or memory

benchmarks are not reported.
6. Sensitivity of performance to the choice and number of observables could be explored more deeply.

3. Comments for Author

1. The paper presents a strong and original contribution to active learning for materials discovery.
2. Clarifying guidelines for constructing observables in new domains would further enhance usability.
3. Including additional experiments on more datasets or tasks would strengthen the generality claims.
4. A brief discussion comparing this approach with multi-objective or Pareto-based active learning would be valuable.
5. Exploring learned or adaptive observables in future work could significantly extend the framework.
6. Overall, the work is technically sound, clearly presented, and impactful.

4. Novelty and Originality

Moderate

5. Overall evaluation

Accept with Minor Revision

Reviewer #2

Questions

1. Strengths of the Paper

The methodology is mathematically grounded, with well-defined uncertainty measures incorporating both variance and cross-observable covariance
Comparison against multiple strong baselines (QBC, EI, BADGE, CoreSet, Random Sampling) strengthens the empirical claims.

2. Shortcomings in the Paper

The framework is validated on two tasks only; broader validation on additional materials datasets would strengthen claim

3. Comments for Author

Consider including runtime and memory benchmarks to complement the sample-efficiency results.
Expand discussion on how observables can be learned automatically rather than manually defined.

4. Novelty and Originality

Moderate

5. Overall evaluation

Accept with Minor Revision

Reviewer #3

Questions

1. Strengths of the Paper

The paper introduces a principled quantum-inspired uncertainty formulation, moving beyond metaphorical use of “quantum” ideas to mathematically grounded constructs

2. Shortcomings in the Paper

Since the method is implemented on classical hardware, some readers may question whether the gains stem from quantum principles or from sophisticated covariance modeling
Methods such as deep ensembles with correlated outputs or multi-task Bayesian neural networks could be relevant baselines

The paper to be edited in IEEE format

3. Comments for Author

Consider adding: Multi-property optimization, Discrete materials classification, Transfer learning across materials families
Identify scenarios where correlated uncertainty may mislead selection (e.g., spurious covariance in noisy regimes

The paper to be edited in IEEE format

4. Novelty and Originality

High

5. Overall evaluation

Accept with Minor Revision