Data-driven multi-objective alloy design and metal up-cycling using machine-learned quantum optimization

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Quantum annealing has the potential to provide practical quantum advantage for complex optimization tasks. Here, we present a systematic assessment of an integrated factorization-machine and quantum-annealing workflow (FM+QA) for a technologically relevant application: multi-objective Pareto optimization in metal up-cycling through alloy design. The data-driven FM+QA active learning scheme is based on iteratively training factorization machine surrogate models on materials data sets in quadratic unconstraint binary optimization (QUBO) form, and solving them with quantum optimization algorithms. To address the non-convex nature of the Pareto front, we employ the recently proposed data-driven Tchebycheff scalarization scheme. We then show that the proposed FM+QA workflow extends the applicability of QUBO-based optimization to data-driven materials design problems with multiple competing objectives.

In particular, we analyze the scaling behavior of the approach and compare quantum annealing with classical simulated annealing, highlighting significant gains in efficiency and solution quality. Furthermore, we provide a critical perspective on the problem sizes and encoding strategies for which quantum-annealing-based optimization may become practically beneficial in the near future. Overall, our results provide foundational blocks for embedding QUBO-based workflows within next-generation computational materials discovery & design pipelines.

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References

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