** Materials Science and Engineering**

122 S. Central Campus Drive, Salt Lake City, Utah 84112 (801) 581-8632

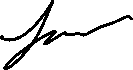
January 7, 2023

Dear Editor:

We are very pleased to submit this data article to Data in Brief. Our manuscript, titled Materials Science Optimization Benchmark Dataset for Multi-fidelity Hard-sphere Packing Simulations provides important research from my research group at the University of Utah. This work presents a benchmark dataset for materials science optimization tasks that incorporates both simulation failure and heteroskedastic noise in a realistically complex setting.

The dataset represents 279 days’ worth of CPU computation time and contains over 400,000 datapoints. The two datasets presented in this work can be used to create a surrogate model as close as possible to running the actual simulations. This will help form part of a larger suite of experimentally and computationally derived benchmarks. Additionally, this dataset can serve as an optimization task for advanced Bayesian optimization topics including multi-fidelity and linearly constrained optimization.

Sincerely,



Dr. Taylor Sparks  
Associate Professor & Associate Chair  
Materials Science and Engineering Department  
University of Utah  
Salt Lake City, Utah 84112