Pseudopotentials for high-throughput DFT calculations

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High-throughput density functional theory (DFT) calculations require a comprehensive set of pseudopotentials or PAWs that are 1) accurate in any realistic material, 2) computationally efficient, and 3) systematically tested. Here, we present the GBRV pseudopotential library[1], optimized for such high-throughput calculations. We present our initial design criteria, testing procedure, and validation. Since the initial publication of our library, there has been been significant progress in the field of pseudopotential design and testing. In light of these works, we discuss changes in the GBRV library over time, updated testing sets and results, and possible future directions for pseudopotential development.

References

[1] K.F. Garrity *et. al.*, Comput. Mater. Sci. **81** 446 (2014)