Automated Generation of Highly Accurate, Efficient and Transferable Pseudopotentials

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A genetic algorithm was used to automate the search for optimized pseudopotential parameters. Genetic algorithms (GA) have been used extensively to solve complex engineering problems with coupled parameters and multiple-minima design spaces. These algorithms can be highly parallelized and are extremely powerful due to the ability to automate the exploration of extremely large search spaces. This proof-of-concept study shows that combining GA with *ab-initio* simulations can produce a Pareto set of pseudopotentials. This family of solutions demonstrates the trade-off between accuracy and computational efficiency. The two objectives chosen were accuracy (compared to a validated work of Holzwarth et. al [1]) and the number of Gflops required for crystal structure calculation. To encourage potential transferability, each element was optimized in three different lattices: 1)nitrogen in GaN, AlN, and YN, 2)oxygen in NO, ZnO, and SiO_4, and 3)fluorine in LiF, NaF, and KF. The optimal solutions generated here are equivalent in accuracy and required significantly less computational work than the validated data of Holzwarth et al[1]. Ultimately, the work presented here shows that GAs can successfully be used to generate a family of highly accurate, efficient, and transferable pseudopotentials.

[1] Holzwarth, N., Tumblston, J., Dellaripa, N., Harris, D., www.wfu.edu/ natalie/papers/pwpaw/periodictable/periodictable.html (2008).