

Abstract Submitted
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Projector Augmented Wave database with automatic parameter optimization¹ R.J. SNOW, University of California Davis, A.F. WRIGHT, Sandia National Laboratory, C.Y. FONG, University of California Davis — Projector Augmented Wave (PAW) parameter sets, similar to pseudopotential parameters, can be constructed in many ways. Due to a non-local expansion of projectors, the PAW method can include parameters for each angular momentum channel separately. While this gives the flexibility to optimize projectors individually, it also creates an unfathomable parameter space for searching for good parameter sets. To automatically search for good PAW sets, logarithmic derivatives were analyzed numerically for matching with AE logarithmic derivatives. Logarithmic derivative matching, total energy convergence, and scf convergence were used as scores for automatic optimization of the accuracy and speed of PAW parameter sets using a genetic algorithm within an optimization code. The Dakota [1] program was used for the parameter optimization, while the atompaw program was used for PAW generation. A new database of PAW functions will be introduced and a number of examples discussed. [1] Sand Report Sand 2001-3514, (2002) [2] N.A.W. Holzwrth, A.R. Tackett, and G.E. Matthews, Computer Physics Communications 135, 329 (2001)

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