

A Projector Augmented Wave (PAW) code for electronic structure calculations – *pwpaw* and *atompaw*¹

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ABSTRACT

The projector augmented wave (PAW) method, developed by Blöchl², is a very powerful tool for performing electronic structure calculations in the local density approximation, combining some of the best features of pseudopotential and all-electron approaches. The *pwpaw* code is an implementation of the PAW method for periodic solids using a plane wave basis. The structure of the program was conceived and developed by Tackett³ in his Ph. D. work on a “real-space” implementation of the PAW formalism. The program is designed to optimize memory and disk access and is user-friendly in the sense that the input file makes good use of keywords and comments. The eigenvalue solvers and self-consistency algorithms are more efficient than those of our earlier work.⁴

The computer program *atompaw* generates projector and basis functions which are needed for the PAW method. We have previously studied several schemes to generate these functions.⁵ The present code uses a procedure similar to that originally suggested by Blöchl, but with a smoother “shape” function which has advantageous convergence properties in Fourier space.

In this poster we present some results of example calculations which illustrate the convergence and accuracy of the calculational method. We are currently preparing the program package for submission to *Computer Physics Communications*.

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²P. E. Blöchl, *Phy. Rev. B* **50**, 17953 (1994).

³A. R. Tackett, *PhD thesis*, Wake Forest University, 1998.

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