

# A Four-Component Relativistic PAW Method

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We are developing an extension of the projector-augmented wave (PAW) method<sup>1,2</sup> to treat relativistic effects including spin-orbit interactions based on a four-component Dirac Hamiltonian. The PAW equations for the large components of the Dirac pseudowavefunctions are Schrödinger-like. The small components are not negligible, but can be accurately determined from the Schrödinger solutions. We present results from atomic calculations to demonstrate the significance of the small component and the accuracy of our approximation.

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- [2] N.A.W. Holzwarth, G.E. Matthews, R.B. Dunning, A.R. Tackett, and Y. Zeng, *Phys. Rev. B* **55**, 4, 2005-2017 (1997); N.A.W. Holzwarth, A.R. Tackett, G.E. Matthews, *Computer Phys. Comm.* **135**, 329-347 and 348-376 (2001).