

Abstract Submitted
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Optimizing Generalized Norm-Conserving Pseudopotentials D.R.

HAMANN, Dept. of Physics & Astronomy, Rutgers University — The “generalized” method permits the construction of norm-conserving pseudopotentials at energies that do not correspond to bound atomic states, giving added flexibility in the treatment of angular-momentum channels for which no bound states exist.¹ An effective method for optimizing the convergence of pseudopotential calculations with plane-wave-basis cutoff energy requires atomic wave functions with decaying tails, and has not been applicable to such “generalized” states.² By introducing a potential well outside the core radius for selected angular-momenta, an artificial decaying tail can be produced for positive-energy states. This permits the application of the optimization method, and we find convergence behavior comparable to that for ordinary bound states. In practice, we terminate the positive-energy all-electron wave function smoothly with an exponential or Gaussian tail, and never need to treat the implied well potential explicitly. The projectors to form fully-nonlocal operators³ can be terminated at the core radii as usual, despite differences of the semi-local potentials outside the well radii.

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²A. M. Rappe, *et al.*, Phys. Rev. B **41**, 1227 (1990).

³L. Kleinman and D. M. Bylander, Phys. Rev. Lett. **48**, 1425 (1982).

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