

Separable dual-space Gaussian pseudopotentials

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We present pseudopotential coefficients for the first two rows of the Periodic Table. The pseudopotential is of an analytic form that gives optimal efficiency in numerical calculations using plane waves as a basis set. At most, seven coefficients are necessary to specify its analytical form. It is separable and has optimal decay properties in both real and Fourier space. Because of this property, the application of the nonlocal part of the pseudopotential to a wave function can be done efficiently with a grid in real space. Real space integration is much faster for large systems than ordinary multiplication in Fourier space, since it shows only quadratic scaling with respect to the size of the system. We systematically verify the high accuracy of these pseudopotentials by extensive atomic and molecular test calculations. [S0163-1829-96104927-2](#)

I. INTRODUCTION

is obtained by modifying existing pseudopotentials of the

Kleinman-Bylander type.

⁴ The Kleinman-Bylander form

initially was intended for real space use and therefore does not satisfy any optimality conditions for real space integration. In contrast to previous work we therefore start out with an analytical form, which has all of the optimality properties with respect to real space integration built in. A small number of parameters is then adjusted in such a way as to reflect the properties of different atoms. In contrast to most (pseudo-)potential calculations the matrix elements can be calculated analytically. The chosen analytical form gives nevertheless

because all the matrix elements can be calculated analytically. The chosen analytical form gives nevertheless

s _____

r _____

$$\frac{r!}{r} \sim \frac{G}{A_G} \cdot \frac{1}{2}$$

They are normalized such that

 $\sim r \quad r$

144.9a1 part

we WbtaQV for the

$$V \sim_K 524p$$

$$p \parallel v \sim \log n^2 \quad K! \#$$

$$\begin{array}{ccccc} ! & \sim & K! & \# & @ \\ & & K! & \sim & K! \end{array}$$

$$\sim_K \not\models (\sim_{\hat{K}} \frac{\sim !h \sim_K !Y}{\sim_K !Y})$$

$$\hat{K} \hat{K} \quad !p_1^p - K!h_1^p p_1^p - K!Y_p^* \sim \quad !, \quad ,m$$

The projectors $p^l_{\mathcal{N}}$

(K) can be calculated analytically and

all the relevant quantities, with respect to the plane wave energy cutoff. The first factor Q is the location of the peak of the pseudo-wave-function. In order to just qualitatively reasonable result, the minimal wavelength represented by Q is $\lambda_Q = 2\pi/Q$. In the case of a periodic potential, Q is the reciprocal lattice vector. In the case of a non-periodic potential, Q is the wave vector of the plane wave.

therefore large for Al and small for Cl. We did not see

well multiple bonds, which typically are shorter than single bonds and therefore more difficult to describe with a pseudopotential. Also molecules, the constituent atoms of which have large differences in electronegativity were preferably chosen. In these cases, the inert region⁹ shrinks considerably, since the atom with the larger electronegativity imposes its electronic structure in regions very close to the nucleus of the less electronegative atom. They are thus the most difficult molecules for treatment with pseudopotentials. Also, in these molecules the bond length deviates very much from what one would obtain by adding the covalent radii.

The results are shown in Table V. We see that the errors for compounds containing the first row atoms B, C, N, O, and F, as well as H, are extremely small. These errors arising from the pseudopotential approximation are of the order of a few thousandths of a Bohr and thus nearly ten times smaller than the errors arising from the LDA approximation. The errors for compounds containing the second row atoms are larger and comparable to the LDA errors. These relatively large errors can be traced back to the relatively shallow outermost core shells of these second row atoms. The errors are

numerical noise, which was very helpful in the minimization procedure. In addition, Q_t can also be calculated much faster numerically. Nevertheless, one can use these pseudopotential parameters with any other LDA parametrization, without changing the results on a relevant scale. The entries in Tables I and II have the following meaning with the notation of the previous sections:

required for response functions, and it is much faster to compute than any other known form. It has the deficiency that the high density limit of correlation is not reproduced, but there are two ameliorating factors. The first is essentially exact for $r=100$, the density at which the response corresponds to $r=100$, the density at which the response corresponds to $r=100$.

This form is based on the following rational polynomial:

xc5201ar_s12r_s^{25 95. +09 Tm(1) Tj/F12 1 Tf0. 913 0 TD1a}

