Switching function

Equations (3.15)–(3.19) in the main paper define the elementary switching function introduced by York and Karplus,\,\footnote{1} which we have adopted for our switching/Gaussian methodology. The parameters $R_{\text{sw},J}$ and $\alpha_J$ (where $J$ indexes atomic spheres) were not completely defined in the paper. These definitions, which we take from Ref. 1, are repeated here for completeness.

If $N_J$ is the number of Lebedev grid points used to discretize the $J$th sphere, whose radius is $R_J$, then the width of the switching region around atom $J$ is defined to be

$$R_{\text{sw},J} = R_J \sqrt{\frac{14}{N_J}} . \tag{S.1}$$

The scaling parameter $\alpha_J$ is defined as

$$\alpha_J = \frac{1}{2} + \frac{R_J}{R_{\text{sw},J}} - \sqrt{\left( \frac{R_J}{R_{\text{sw},J}} \right)^2 - \frac{1}{28}} . \tag{S.2}$$

These two equations complete the definitions of $R_{\text{in},J}$ and $R_{\text{out},J}$, the inner and outer boundaries of the switching region for atom $J$. Note that the penetration depth, $d_{i,J}$, which we defined in Eq. (3.17), is the same quantity that York and Karplus denote by $\hat{r}_{i,J}$.

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2 Convergence data

Figures 4 and 5 in the paper depict various tests of convergence with respect to the number of Lebedev grid points per atomic sphere, $N$. (We use the same $N_J$ for all $J$.) It may be useful to see the actual numerical data, in order to get a sense of the error associated with a particular value of $N$. Table I provides these data. (Recall that the data set consists of the 20 amino acids.)

References

Table S1: Mean values of the rotational variance ($\Delta_{\text{rot}}$), energy and gradient discretization errors, and Gauss’ Law error ($\Delta_{\text{GL}}$), as a function of the number of Lebedev grid points per atom. Values in parentheses are standard deviations over the set of 20 amino acids. The Gauss’ Law error is not computed for the Hartree-Fock (HF) calculations, since not all of the solute charge is contained within the cavity. In evaluating the energy and gradient discretization errors, the result with $N = 1202$ is taken to represent the exact result.