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Molecular Finite Element Density Functional Calculations employing a Cusp Factor

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Finite element calculations have been performed in Cartesian coordinates using the density functional approach
for a number of small molecules. In order to aid convergence
of the orbitals and total energies a suitable cusp factor was employed, such that the resulting effective potential is non-singular at all nuclei. The resulting total energies
and densities were compared with those obtained using the Gaussian basis set package NWChem and excellent agreement was found.

Apply to be
 considered for a student
   award (Yes / No)?

N/A

Level for award
 (Hons, MSc,
   PhD, N/A)?

N/A

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