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Improved forces and nonlocal operators using high- order integration[1] GRADY SCHOFIELD, N. SCOTT BOBBITT, CHARLES LENA, JAMES R. CHELIKOWSKY, University of Texas at Austin — We present a new high-order modification to the finite-difference based real space pseudopotential density functional theory method. By giving a high-order treatment to the nonlocal pseudopotential terms in the Hamiltonian, as well as all quantities of interest obtained by post-processing the wavefunctions, we improve the accuracy of total energy, interatomic forces, vibrational modes, and anharmonic effects. We demonstrate the power of this new technique by computing vibrational modes for a few common molecules containing atoms that are more difficult for high-accuracy force calculations, such as oxygen and nitrogen, due to the depth of the pseudopotential. The reduction in numerical noise as atoms move over the grid allows using a larger grid spacing than would be required with a conventional finite difference based discretization. Savings in both memory and computational time, due to a smaller spectral radius, will be discussed.

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