Atomic Forces and Geometry Optimisation with the ONETEP Linear-Scaling DFT Method

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ONETEP uses a localised yet orthogonal basis of periodic cardinal sine (psinc) functions[2], also known as Dirichlet or Fourier Lagrange-mesh functions, which are formed from a discrete sum of plane-waves. The localised non-orthogonal generalised Wannier functions (NGWFs) which span the occupied subspace are represented in terms of these psinc functions and are optimised during the calculation. This choice of basis and optimisation of the NGWFs results in smooth potential energy surfaces and enables the use of the Hellmann-Feynman theorem for the calculation of atomic forces. These have been implemented within a quasi-Newton geometry optimisation scheme and preliminary results are presented.