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Optimised local orbitals from linear-scaling density-functional theory calculations PETER HAYNES, LAURA RATCLIFF, Imperial College London, GARETH CONDUIT, Weizmann Institute of Science, PHILIP AVRAAM, Imperial College London, MARK ROBINSON, University of Cambridge — Total energy calculations within density-functional theory can be performed with a computational cost that scales linearly with system-size by employing a density-matrix-based description of the fictitious Kohn-Sham system and exploiting the property of nearsightedness. One class of linear-scaling methods determines the ground-state density-matrix by optimising a set of local orbitals in situ, as for example implemented in the ONETEP code, where they are referred to as "nonorthogonal generalised Wannier functions". This work investigates the physical significance of such orbitals and assesses whether the term Wannier function is appropriate. Band structures interpolated from these orbitals are presented and compared with those from traditional methods. It is seen that the occupied valence and low-lying conduction bands are well-described, but that states higher up in energy in the conduction band are poorly described or even absent. Changes in macroscopic polarisation are also calculated using a generalisation of the centre of charge to the nonorthogonal case.

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