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ONETEP: linear-scaling density-functional theory with plane waves PETER HAYNES, Cavendish Laboratory, University of Cambridge, UK, CHRIS-KRITON SKYLARIS, Physical and Theoretical Chemistry Laboratory, University of Oxford, UK, ARASH MOSTOFI, Department of Materials Science and Engineering, Massachusetts Institute of Technology, MIKE PAYNE, Cavendish Laboratory, University of Cambridge, UK — Plane waves are a popular choice of basis set for first-principles quantum-mechanical simulations based on density-functional theory because the implementation is straightforward and the completeness can be controlled systematically with a single parameter. The resulting simulations require a computational effort which scales as the cube of the system-size, which makes the cost of large-scale calculations prohibitive. Extended basis functions would appear to be an inappropriate choice for expanding the localized orbitals of linear-scaling methods or for embedding the calculation within a larger model. In spite of these apparent difficulties, the ONETEP linear-scaling method can achieve the same accuracy as traditional plane-wave calculations and overcomes the apparent difficulties mentioned above. An outline of the ONETEP method will be presented, focusing on its distinctive features and primarily the ability to optimize the localized orbitals in each particular environment. These optimized orbitals are known as non-orthogonal generalized Wannier functions within ONETEP, and justification for this term will be presented, in addition to results that demonstrate the scaling and accuracy of the method.

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