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Practical techniques for order−N DFT calculations on thousands of atoms

D. Bowler, T. Miyazaki and M. J. Gillan

Physics and Astronomy Dept., University College London Gower Street, London WC1E 6BT, United Kingdom

Despite the extraordinary success of density functional calculations in fields as diverse as physics, chemistry, geology and biology, there is still a major bottleneck in conventional approaches: the computational effort scales with the square of the number of atoms treated, and asymptotically as the cube of the number of atoms. This has limited practical calculations to about a thousand atoms. Over the last few years, there has been a major effort to develop codes that scale linearly with the number of atoms: order−N techniques. We will describe the theory behind our code CONQUEST, and its implementation on massively parallel machines, emphasizing not only that it is a full ab initio method, but also that it is capable of accuracy equivalent to that of standard plane−wave methods. We will present illustrative results of work in which CONQUEST is used to perform self−consistent DFT calculations on systems containing over ten thousand atoms.