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Recent Progress in Linear Scaling DFT

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Linear scaling or O(N) electronic structure codes have been under development for around fifteen years. After an initial explosion of interest, the practical difficulties of implementation and efficiency have led to a slow down in development and applications. In this talk I will present details of recent developments in the massively parallel CONQUEST linear scaling DFT code, and make some comments on the linear scaling field in general. The CONQUEST code is one of the leading O(N) codes, and has demonstrated not only excellent scaling to over two million atoms and many thousands of cores but also practical applications to nanostructures on semiconductor surfaces, and recently to biological systems. I will describe the details of the CONQUEST code, including recent developments in basis functions and parallelisation. I will also discuss recent improvements including constrained DFT, exact exchange and TDDFT, all of which have been implemented with linear scaling.

D. R. Bowler and T. Miyazaki, Rep. Prog. Phys. **75** 036503 (2012).