Towards large-scale accurate Kohn-Sham DFT for the cost of tight-binding

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We present recent, and ongoing, work aimed at highly accurate calculations for large-scale systems. The implementation of the *filtration* method [1,2,3] in the `AIMPRO` Gaussian orbital code is described. Timings and accuracy results are presented for defective semiconducting and metallic systems and a range of quantities, such as formation energies, forces, relaxed structures, vibrational modes and free energies. For example, the time taken to calculate a self-consistent total energy of 1000 silicon atoms (to achieve an average error of less than 10^{-4} angstrom in relaxed structures) is shown to be currently possible in less than 30 minutes on a single 2.8 GHz Intel i7 core.

We finish with a summary of realistic near-term aims, most notably an aim which can be summarised as 'plane-wave accuracy for the cost of a tight-binding calculation'.

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