

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Auxiliary density functionals: a new class of methods for efficient, stable density functional theory calculations¹ PHIL HASNIP, MATT PROBERT, University of York — *Ab initio* materials modelling methods have become an essential tool for physical scientists in a wide variety of fields. The advent of more and more powerful computers has allowed larger, more complex systems to be simulated and the dramatic improvements in both experimental growth and characterisation methods have allowed the length scale of theoretical simulations and experimental studies to coincide at the nanoscale. Whilst there has been undoubted success in the modelling of nanomaterials, the approach is not without its problems. As the size of the simulation system is increased, the conventional algorithms used to find the electronic ground state often show poor convergence, and for large or complex systems they may fail to converge at all. We present a new class of methods for solving the Kohn-Sham equations based on constructing a mapping dynamically between the Kohn-Sham system and an auxiliary system. This auxiliary system is not required to be fermionic, and an exemplar bosonic scheme is presented which captures the key features of the Kohn-Sham behaviour. This auxiliary scheme is shown to provide good performance for a variety of bulk materials, and a substantial improvement in the scaling of calculations with system size for a range of materials.

¹Supported by the United Kingdom Car-Parrinello Consortium (UKCP) and EPSRC (grant ref. EP/K013564/1).

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Date submitted: 14 Nov 2014

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